A mathematical analysis of the GW^0 method for computing electronic excited energies of molecules

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Abstract

This paper analyses the GW method for finite electronic systems. In a first step, we provide a mathematical framework for the usual one-body operators that appear naturally in many-body perturbation theory. We then discuss the GW equations which construct an approximation of the one-body Green's function, and give a rigorous mathematical formulation of these equations. Finally, we study the well-posedness of the GW^0 equations, proving the existence of a unique solution to these equations in a perturbative regime.

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1 Introduction

Computational quantum chemistry is nowadays a standard tool to numerically determine the properties of molecules. The Density Functional Theory (DFT) first developed by Hohenberg and Kohn [20] and by Kohn and Sham [25], is a very powerful method to obtain ground state properties of molecular systems. However, it does not allow one to compute optical properties and electronic excited energies. In order to calculate such quantities, several approaches have been considered in the last decades [31]. Among them are the time-dependent DFT (TDDFT) [28, 29], wave-function methods [19] such as Coupled-Cluster, full-CI and Green's function methods. In this article, we study the GW method, which is based on Hedin's equations for the one-body Green's function [18]. The formal derivation of the latter equations relies on many-body perturbation techniques. While the GW method has been proven very successful in practice to predict electronic-excited energies, no rigorous mathematical framework has yet been developed to understand its mathematical properties. The aim of this work is to present such a framework.

In non-relativistic first-principle molecular simulation, the electrons of a molecular system are described by an N-body Hamiltonian operator H_N, which is a bounded below self-adjoint operator on the fermionic space $\bigwedge^N L^2(\mathbb{R}^3)$ (see Equation (30) below). Whenever $N \leqslant Z$, where Z is the total nuclear charge of the molecular system, H_N has an infinity of discrete eigenvalues $E_N^0 \leqslant E_N^1 \leqslant E_N^2 \leqslant \cdots$ below the bottom of the essential spectrum, where E_N^0 is its ground state energy. The quantities we would like to evaluate are the *electronic-excitation energies*

$$E_N^0 - E_{N+1}^k \quad \text{(gain of an electron)}, \quad \text{and} \quad E_N^0 - E_{N-1}^k \quad \text{(loss of an electron)}.$$

These energy differences are not to be confused with the optical-excitation energies, which are energy differences of the form $E_N^k - E_N^0$, between two states with the same number of electrons. More generally, it is interesting to compute the particle electronic-excitation set $S_{\rm p} := \sigma\left(H_{N+1} - E_N^0\right)$ and the hole electronic-excitation set $S_{\rm h} := \sigma\left(E_N^0 - H_{N-1}\right)$. As will be made clear in Section 3.2, these sets are closely linked to the one-body Green's function: the time-Fourier transform of the Green's function becomes singular on these sets. In order to study the electronic-excitation sets, we therefore study the one-body Green's function. Also, the one-body Green's function is a fundamental object which contains a lot of useful information, and allows one to easily compute the ground state electronic density, the ground state one-body density matrix, and even the ground state energy thanks to the Galitskii-Migdal formula [15].

Calculating the one-body Green's function is however a difficult task. In his pioneering work in 1965, Hedin proved that the Green's function satisfies a set of (self-consistent) equations, now called the Hedin's equations [18]. These equations link many operator-valued distributions, namely the reducible and irreducible polarizability operators, the dynamically screened interaction operator, the self-energy operator, the vertex operator, and of course the one-body Green's function. The state-of-the-art method to compute the one-body Green's function consists in solving Hedin's equations.

Immediately, two difficulties arise. The first one is related to the lack of regularity of the Green's function (we expect its time-Fourier transform $\widehat{G}$ to be singular on the electronic-excitation sets). One way to get around this problem is to consider the analytical extension of $\widehat{G}$ into the complex plane, which we denote by $\widetilde{G}$. This is possible whenever the following classical stability condition holds true[1]:

> **Stability assumption:** It holds that $2E_N^0 < E_{N+1}^0 + E_{N-1}^0$.

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[1] The question "Is the stability condition always true for Coulomb systems" is still an open problem [3, Part VII].

The physical relevance of this inequality is discussed for instance in [11, Section 4.2]. It allows one to define the chemical potential μ, chosen such that

$$E_N^0 - E_{N-1}^0 < \mu < E_{N+1}^0 - E_N^0.$$

Instead of studying the Green's function $G(\tau)$ in the time domain, or its Fourier transform $\widehat{G}(\omega)$ in the frequency domain, we rather study its analytical continuation $\widetilde{G}$ on the imaginary axis $\mu + \mathrm{i}\mathbb{R}$. The function $\omega \mapsto \widetilde{G}(\mu + \mathrm{i}\omega)$ enjoys very nice properties, both in terms of regularity and integrability, which makes it a privileged tool for numerical calculations.

The second difficulty comes from the fact that Hedin's equations cannot be exactly solved and, even more importantly, that the mathematical definition of some terms in these equations are unclear. It however opens the way to some approximate resolutions. The most widely used approximation nowadays is the so-called GW-approximation, also introduced by Hedin [18]. These equations are traditionally set on the time-axis, or on the energy-axis [37, 26]. However, as previously mentioned, the various operators under consideration are singular on these axes, which makes the traditional GW equations cumbersome to implement numerically, and difficult to analyze mathematically. In order to manipulate better-behaved equations, it is more convenient to replace every operator-valued distribution involved in the GW equations by its analytic continuation on an appropriate imaginary axis, thanks to the "contour deformation" technique introduced in [36, 34]. The resulting GW equations, which give an approximation of the map $\omega \mapsto \widetilde{G}(\mu + \mathrm{i}\omega)$, turn out to give simulation results in very good agreement with experimental data [41, 42, 7, 8].

From the GW equations set on the imaginary axis, several further approximation may be performed. The GW equations are solved self-consistently, and the Green's function is updated at each iteration until convergence. When only one iteration is performed, we obtain the one-shot GW approximation, also called the $\mathrm{G}_0\mathrm{W}^0$ approximation of the Green's function. For molecules, self-consistent GW approaches give results of similar quality as $\mathrm{G}_0\mathrm{W}^0$, sometimes almost identical [42, 26], sometimes slightly worse [37], sometimes slightly better [7, 8]. When several iterations are performed, while keeping the screening operator W fixed, equal to a reference screening operator W^0, we obtain the GW^0 approximation of the Green's function [42, 46]. Since the update of the screening operator W in a self-consistent GW scheme seems difficult to analyze mathematically, we prefer to study in this article the equations resulting from the GW^0 approximation.

The purpose of this article is threefold. First, we clarify the mathematical definitions and properties of the usual one-body operators involved in many-body perturbation theory. Then, we embed the GW^0 equations in a mathematical framework. Finally, we prove that, in a perturbative regime, the GW^0 equations admit a unique solution close to a reference Green's function.

From a physical viewpoint, the analysis we perform in this work is more relevant for atoms and molecules. Indeed, as discussed in [5, Section 4.1] for instance, fully self-consistent GW approaches are questionable for solid-state systems, for which quasiparticle methods are preferred [1, 2].

The paper is organized as follows. In Section 2, we provide the mathematical tools that will be used throughout the article. We recall the Titchmarsh's theorem, and introduce the kernel-product of two operators, which can be seen as an infinite dimensional version of the Hadamard product for matrices. We also explain the underlying structure that makes the "contour deformation" possible. In Section 3, we recall the standard definitions of the usual one-body operators that appear in many-body perturbation theory. A consistent functional setting is given for each of these operators, and their basic properties are recalled and proved. Section 4 is concerned with the GW approximation. We explain why some of the GW equations are not well-understood mathematically, and prove that the GW^0 equations are well-posed in a perturbative regime. Most of the proofs are postponed until Section 6.

2 Setting the stage

2.1 Some notation

The GW method is based on time-dependent perturbation theory and therefore involves space-time operators. Following the common notation in physics, we denote by t the time coordinate, by $\mathbf{r}$ the space coordinates, and by $\mathbf{x}$ or $\mathbf{r}t$ the space-time coordinates. The functional spaces considered in this work are by default composed of complex-valued functions, unless we explicitly mention that the functions are real-valued.

Most of the space-time operators appearing in the GW formalism are time-translation invariant. A time-translation invariant operator $\mathcal{C}$ can be characterized by the family of operators $(C(\tau))_{\tau \in \mathbb{R}}$ such that, formally, the kernel of $\mathcal{C}$ is of the form $\mathcal{C}(\mathbf{r}_1 t_1, \mathbf{r}_2 t_2) = C(\mathbf{r}_1, \mathbf{r}_2, t_1 - t_2)$, where $C(\mathbf{r}, \mathbf{r}', \tau)$ is the kernel of the operator $C(\tau)$. For clarity, we will systematically use the letter τ to denote a time variable which is in fact a time difference.

Let $\mathcal{H}$ be a separable complex Hilbert space, whose associated scalar product is simply denoted by $\langle \cdot, \cdot \rangle$ and the associated norm $\| \cdot \|$. We denote by $\mathcal{B}(\mathcal{H})$ the space of bounded linear operators on $\mathcal{H}$, by $\mathcal{S}(\mathcal{H})$ the space of bounded self-adjoint operators on $\mathcal{H}$, by $\mathfrak{S}_p(\mathcal{H})$ ($1 \leqslant p < \infty$) the Schatten class

$$\mathfrak{S}_p(\mathcal{H}) = \left\{ A \in \mathcal{B}(\mathcal{H}) \ \middle| \ \|A\|_{\mathfrak{S}_p(\mathcal{H})} := \mathrm{Tr}(|A|^p)^{1/p} < \infty \right\},$$

and by A^* the adjoint of a linear operator A on $\mathcal{H}$ with dense domain. The real and imaginary parts of an operator $A \in \mathcal{B}(\mathcal{H})$ are defined as

$$\mathrm{Re}\, A = \frac{A + A^*}{2}, \quad \mathrm{Im}\, A = \frac{A - A^*}{2\mathrm{i}}.$$

Note that, when A is closed (which implies $A^{**} = A$), the operators $\mathrm{Re}\, A$ and $\mathrm{Im}\, A$ are self-adjoint. For $f, g \in \mathcal{H}$ and given operators A, B on $\mathcal{H}$, we will often use the notation

$$\langle f|A|g \rangle_{\mathcal{H}} := \langle f, Ag \rangle_{\mathcal{H}}, \qquad \langle f|AB|g \rangle_{\mathcal{H}} := \langle f, ABg \rangle_{\mathcal{H}},$$

even in cases when the operators are not self-adjoint. Operators are always understood to act on the function on the right in this notation.

We will sometimes need to manipulate the adjoints of operators between two different Hilbert spaces $\mathcal{H}_a$ and $\mathcal{H}_b$. The adjoint of a bounded operator $A \in \mathcal{B}(\mathcal{H}_a, \mathcal{H}_b)$ is the bounded operator $A^* \in \mathcal{B}(\mathcal{H}_b, \mathcal{H}_a)$ defined by

$$\forall (x, y) \in \mathcal{H}_a \times \mathcal{H}_b, \qquad (A^* y, x)_{\mathcal{H}_a} = (y, Ax)_{\mathcal{H}_b}.$$

Let E be a Banach space. We denote by $\mathscr{S}'(\mathbb{R}, E)$ the space of E-valued tempered-distributions on $\mathbb{R}$, *i.e.* the set of continuous linear maps from the Schwartz's functional space $\mathscr{S}(\mathbb{R})$ into E. Recall that, by definition, a family $(T_\eta)_{\eta > 0}$ of elements of $\mathscr{S}'(\mathbb{R}, E)$ converges in $\mathscr{S}'(\mathbb{R}, E)$ to some $T \in \mathscr{S}'(\mathbb{R}, E)$ when η goes to 0 if

$$\forall \phi \in \mathscr{S}(\mathbb{R}), \qquad \|\langle T_\eta, \phi \rangle_{\mathscr{S}', \mathscr{S}} - \langle T, \phi \rangle_{\mathscr{S}', \mathscr{S}} \|_E \xrightarrow[\eta \to 0^+]{} 0.$$

Let $f \in L^1(\mathbb{R}, E)$ be a time-dependent E-valued integrable function. The time-Fourier transform of f is defined, using the standard convention in physics, as

$$\forall \omega \in \mathbb{R}, \quad \widehat{f}(\omega) := (\mathcal{F}_T f)(\omega) := \int_{\mathbb{R}} f(\tau) \mathrm{e}^{\mathrm{i}\omega\tau} \, \mathrm{d}\tau. \tag{1}$$

For the sake of clarity, we will sometimes denote by $\mathbb{R}_t$ or $\mathbb{R}_\tau$ the time-domain, by $\mathbb{R}_\omega$ the frequency-domain, by $\mathscr{S}'(\mathbb{R}_\tau, E)$ (resp. $\mathscr{S}'(\mathbb{R}_\omega, E)$) the space of time-dependent (resp. frequency-dependent) E-valued distributions, etc. We will also denote with a hat the functions defined on the frequency

domain. Using this notation, $\mathcal{F}_T$ can be extended to a bicontinuous isomorphism from $\mathscr{S}'(\mathbb{R}_\tau, E)$ into $\mathscr{S}'(\mathbb{R}_\omega, E)$. When $\widehat{f} \in L^1(\mathbb{R}_\omega, E)$, we have

$$\forall \tau \in \mathbb{R}, \quad \left(\mathcal{F}_T^{-1} \widehat{f} \right)(\tau) = \frac{1}{2\pi} \int_\mathbb{R} \widehat{f}(\omega) \mathrm{e}^{-\mathrm{i}\omega\tau} \, \mathrm{d}\omega.$$

The Dirac distribution at $a \in \mathbb{R}^d$ is denoted by δ_a, and the Heaviside function on $\mathbb{R}$ by Θ:

$$\Theta(\tau) = 1 \text{ for } \tau > 0, \qquad \Theta(\tau) = 0 \text{ for } \tau < 0, \qquad \Theta(0) = 1/2. \tag{2}$$

Recall that the time-Fourier transform of Θ is, in the tempered distributional sense,

$$\widehat{\Theta}(\omega) = \pi\delta_0(\omega) + \mathrm{i}\,\mathrm{p.v.}\left(\frac{1}{\omega}\right), \tag{3}$$

where p.v. is the Cauchy principal value. We will also make use of the notation τ^+ for a number strictly above τ, but infinitesimally close to τ, and of the convention

$$\Theta(\tau)\delta_0(\tau^+) := \delta_0(\tau), \quad \Theta(-\tau)\delta_0(\tau^+) := 0.$$

2.2 Hilbert transform of functions and distributions

The Hilbert transform, which amounts to a convolution by $\pi^{-1}\mathrm{p.v.}(\frac{1}{\cdot})$, plays a crucial role in the GW formalism. We first recall some well-known results on the standard Hilbert transform on $L^p(\mathbb{R}_\omega)$, and extend the results to the Sobolev spaces $H^s(\mathbb{R}_\omega)$ for $s \in \mathbb{R}$. Usually, the name "Hilbert transform" is only used on functional spaces $E \subset L^1_{\mathrm{loc}}(\mathbb{R}_\omega)$ such that, for any function $\widehat{f} \in E$, the limit

$$\left[\widehat{f} * \mathrm{p.v.}\left(\frac{1}{\cdot}\right) \right](\omega) = \mathrm{p.v.} \int_{-\infty}^{+\infty} \frac{\widehat{f}(\omega')}{\omega - \omega'} \, \mathrm{d}\omega' := \lim_{\eta \to 0^+} \int_{\mathbb{R} \setminus [\omega-\eta, \omega+\eta]} \frac{\widehat{f}(\omega')}{\omega - \omega'} \, \mathrm{d}\omega'$$

exists for almost all $\omega \in \mathbb{R}_\omega$. However, in the sequel, we will also use the name "Hilbert transform" in functional spaces where the above integral representation is not always valid (for instance when $\widehat{f}$ is not a locally integrable function). Note that we define the Hilbert transform on Fourier transforms of functions (*i.e.* on functions on the frequency domain) since this is the typical setting in the GW formalism.

2.2.1 Hilbert transform in L^p spaces

We first begin with the following classical definition (see for instance [17, Section 4.1]).

Definition 1 (Hilbert transform on $\mathscr{S}(\mathbb{R}_\omega)$)**.** *The Hilbert transform of a function $\widehat{\phi} \in \mathscr{S}(\mathbb{R}_\omega)$ is defined by*

$$\mathfrak{H}\widehat{\phi} := \frac{1}{\pi}\mathrm{p.v.}\left(\frac{1}{\cdot}\right) * \widehat{\phi}, \tag{4}$$

or equivalently by

$$\mathfrak{H}\widehat{\phi} := \left(\mathcal{F}_T(-\mathrm{i}\,\mathrm{sgn}(\cdot)) \, \mathcal{F}_T^{-1} \right) \widehat{\phi}, \tag{5}$$

where p.v. $\left(\frac{1}{\cdot}\right)$ *is the Cauchy principal value of the function $\omega \mapsto \frac{1}{\omega}$, $*$ the convolution product, $\mathcal{F}_T$ the Fourier transform defined in (1) and $-\mathrm{i}\,\mathrm{sgn}(\cdot)$ the multiplication operator by the L^∞ function $t \mapsto -\mathrm{i}\,\mathrm{sgn}(t)$ (where $\mathrm{sgn}(t) = \Theta(t) - \Theta(-t)$ is the sign function).*

The Hilbert transform can be extended by continuity to a large class of tempered distributions. We refer to [17, 35] for a proof of the following theorem.

Theorem 2. *For all $\widehat{f} \in L^p(\mathbb{R}_\omega)$ with $1 < p < \infty$, the Hilbert transform*

$$\mathfrak{H}\widehat{f}(\omega) = \text{p.v.} \int_{-\infty}^{\infty} \frac{\widehat{f}(\omega')}{\omega - \omega'} \, d\omega'$$

is well-defined for almost all $\omega \in \mathbb{R}$. It holds $\mathfrak{H} \in \mathcal{B}(L^p(\mathbb{R}_\omega))$ with

$$\|\mathfrak{H}\|_{\mathcal{B}(L^p(\mathbb{R}_\omega))} = \left| \begin{array}{ll} \tan(\pi/(2p)) & \text{if } 1 < p \leqslant 2, \\ \cot(\pi/(2p)) & \text{if } 2 \leqslant p < \infty. \end{array} \right.$$

Moreover, the Hilbert transform commutes with the translations and the positive dilations, and anticommutes with the reflexions. Finally, it is a unitary operator on $L^2(\mathbb{R}_\omega)$.

2.2.2 Hilbert transform in Sobolev spaces

Recall that for any $s \in \mathbb{R}$, the Sobolev space $H^s(\mathbb{R}_\omega)$ is the Hilbert space defined as

$$H^s(\mathbb{R}_\omega) := \left\{ \widehat{f} \in \mathscr{S}'(\mathbb{R}_\omega)) \ \middle| \ (1 + |\cdot|^2)^{s/2} \mathcal{F}_T^{-1} \widehat{f} \in L^2(\mathbb{R}_\tau) \right\},$$

and endowed with the scalar product

$$\left\langle \widehat{f}, \widehat{g} \right\rangle_{H^s} = 2\pi \int_{-\infty}^{+\infty} (1 + \tau^2)^s \overline{(\mathcal{F}_T^{-1} \widehat{f})(\tau)} \, (\mathcal{F}_T^{-1} \widehat{g})(\tau) \, d\tau,$$

and that $H^{-s}(\mathbb{R}_\omega)$ can be identified with the dual of $H^s(\mathbb{R}_\omega)$ when the space $L^2(\mathbb{R}_\omega) = H^0(\mathbb{R}_\omega)$ is used as a pivoting space. One of the reasons to introduce these spaces is that the image of $L^\infty(\mathbb{R}_\tau)$ by the Fourier transform $\mathcal{F}_T$ is contained in the Sobolev spaces of indices strictly lower than $-1/2$.

Lemma 3 (Fourier transform in $L^\infty(\mathbb{R}_\tau)$). *Let $s > 1/2$. Then $\mathcal{F}_T(L^\infty(\mathbb{R}_\tau)) \subset H^{-s}(\mathbb{R}_\omega)$ and*

$$\|\mathcal{F}_T\|_{\mathcal{B}(L^\infty, H^{-s})} = C_s \quad \text{with} \quad C_s = \left(2\pi \int_{\mathbb{R}} \frac{d\tau}{(1 + \tau^2)^s} \right)^{1/2}. \tag{6}$$

For completeness, we recall the proof of Lemma 3 in Section 6.1.

Since the Hilbert transform in $\mathscr{S}(\mathbb{R}_\omega)$ amounts to a multiplication by the bounded function $-i \, \text{sgn}(\cdot)$ in the time domain (see (5)), it can be directly extended to the Sobolev spaces $H^s(\mathbb{R}_\omega)$.

Lemma 4. *For any $s \in \mathbb{R}$, the Hilbert transform $\mathfrak{H}$ is a unitary operator on the Sobolev spaces $H^s(\mathbb{R}_\omega)$ satisyfing $\mathfrak{H}^{-1} = -\mathfrak{H}$ (and therefore $\mathfrak{H}^2 = -\text{Id}$).*

Remark 5 (Hilbert transform of distributions). *Extending the Hilbert transform to Sobolev spaces is straightforward using (5). Extensions of the Hilbert transform to other subspaces of $\mathscr{D}'(\mathbb{R}_\omega)$, such as the $\mathscr{D}'_{L^p}(\mathbb{R}_\omega)$ spaces defined in [38, Section VI.8], can be obtained from (4).*

2.2.3 Hilbert transforms of operator-valued distributions

We now need to properly define the Hilbert transform of operator-valued distributions on the frequency domain, as such objects naturally appear in the GW formalism. We first introduce, for $s \in \mathbb{R}$, the Banach space

$$H^s(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H})) := \left\{ \widehat{A} \in \mathscr{S}'(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}))) \ \middle| \ (1 + |\cdot|^2)^{s/2} \mathcal{F}_T^{-1} \widehat{A} \in L^2(\mathbb{R}_\tau, \mathcal{B}(\mathcal{H})) \right\},$$

endowed with the norm

$$\left\| \widehat{A} \right\|_{H^s(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}))} = \sqrt{2\pi} \left(\int_{-\infty}^{+\infty} (1 + \tau^2)^s \left\| \left(\mathcal{F}_T^{-1} \widehat{A} \right)(\tau) \right\|_{\mathcal{B}(\mathcal{H})}^2 \, d\tau \right)^{1/2}.$$

The following definition makes sense in view of Lemma 4.

Definition 6 (Hilbert transforms of frequency-dependent operators)**.** *Let $\mathcal{H}$ be a Hilbert space, and consider $s \in \mathbb{R}$ and $\widehat{A} \in H^s(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}))$. The Hilbert transform of $\widehat{A}$ is the element of $H^s(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}))$, denoted by $\mathfrak{H}(\widehat{A})$, and defined by*

$$\forall (f,g) \in \mathcal{H} \times \mathcal{H}, \qquad \left\langle f \left| \mathfrak{H}(\widehat{A}) \right| g \right\rangle = \mathfrak{H}\left(\left\langle f \left| \widehat{A} \right| g \right\rangle \right). \tag{7}$$

In particular, it is possible to define the Hilbert transform of the Fourier transform of a uniformly bounded field of time-dependent operators, using the following result, which is a straightforward extension of Lemma 3.

Lemma 7. *Let $\mathcal{H}$ be a Hilbert space, and let $s > 1/2$. Then for all $A \in L^\infty(\mathbb{R}_\tau, \mathcal{B}(\mathcal{H}))$, we have $\widehat{A} \in H^{-s}(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}))$, with*

$$\left\| \widehat{A} \right\|_{H^{-s}(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}))} = \left(2\pi \int_{\mathbb{R}} \left(1 + \tau^2 \right)^{-s} \| A(\tau) \|_{\mathcal{B}(\mathcal{H})}^2 \, \mathrm{d}\tau \right)^{1/2} \leqslant C_s \, \| A \|_{L^\infty(\mathbb{R}_\tau, \mathcal{B}(\mathcal{H}))},$$

where C_s is defined in (6).

Let $\mathscr{B}(\mathbb{R})$ be the set of Borel subsets of $\mathbb{R}$, $b \in \mathscr{B}(\mathbb{R})$ a Borelian set, and H a self-adjoint operator on a Hilbert space $\mathcal{H}$. We denote by $P_b^H := \mathbb{1}_b(H)$ the spectral projection on b of H (here, $\mathbb{1}_b$ is the characteristic function of the set b, and $\mathbb{1}_b(H) \in \mathcal{B}(\mathcal{H})$ is defined by the spectral theorem for self-adjoint operators; see for instance [33, Theorem VII.2]).

Definition 8 (Principal value of the resolvent of a self-adjoint operator)**.** *Let H be a self-adjoint operator on a Hilbert space $\mathcal{H}$. We define the $\mathcal{B}(\mathcal{H})$-valued distribution $\mathrm{p.v.}\left(\frac{1}{\cdot - H} \right)$ on the frequency domain $\mathbb{R}_\omega$ by*

$$\forall (f,g) \in \mathcal{H} \times \mathcal{H}, \qquad \left\langle f \left| \mathrm{p.v.}\left(\frac{1}{\cdot - H} \right) \right| g \right\rangle := \pi \, \mathfrak{H}(\mu_{f,g}^H),$$

where $\mu_{f,g}^H$ is the finite complex Borel measure on $\mathbb{R}_\omega$ defined by

$$\forall b \in \mathscr{B}(\mathbb{R}_\omega), \qquad \mu_{f,g}^H(b) = \langle f | P_b^H | g \rangle.$$

As any complex-valued bounded Borel measure on $\mathbb{R}_\omega$ is an element of $H^{-s}(\mathbb{R}_\omega)$ for any $s > 1/2$ (this is a consequence of the continuous embedding $H^s(\mathbb{R}_\omega) \hookrightarrow C^0(\mathbb{R}_\omega) \cap L^\infty(\mathbb{R})$ for $s > 1/2$), it follows from Definitions 6 and 8 that

$$\mathrm{p.v.}\left(\frac{1}{\cdot - H} \right) = \pi \, \mathfrak{H}(P^H) \quad \text{in } H^{-s}(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H})), \quad s > 1/2,$$

which is the operator analog of the well-known formula

$$\mathrm{p.v.}\left(\frac{1}{\cdot} \right) = \pi \, \mathfrak{H}(\delta_0) \quad \text{in } H^{-s}(\mathbb{R}_\omega), \quad s > 1/2, \tag{8}$$

which is itself a simple reformulation of the equality

$$\mathcal{F}_T^{-1}\left[\mathrm{p.v.}\left(\frac{1}{\cdot} \right) \right] = -\frac{\mathrm{i}}{2} \, \mathrm{sgn}(\cdot) \quad \text{in } L^\infty(\mathbb{R}_\tau).$$

2.3 Causal and anti-causal operators

The GW formalism makes use of families of time-dependent operators $(T_{\mathrm{c}}(\tau))_{\tau \in \mathbb{R}}$ and $(T_{\mathrm{a}}(\tau))_{\tau \in \mathbb{R}}$ of the form

$$T_{\mathrm{c}}(\tau) = \Theta(\tau) A_{\mathrm{c}}(\tau) \quad \text{and} \quad T_{\mathrm{a}}(\tau) = \Theta(-\tau) A_{\mathrm{a}}(\tau),$$

where $\Theta : \mathbb{R} \to \mathbb{R}$ is the Heaviside function (2), and A_{c} and A_{a} belong to $L^\infty(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ for a given Hilbert space $\mathcal{H}$. The family of operators $(T_{\mathrm{c}}(\tau))_{\tau \in \mathbb{R}}$ is called a *causal operator*, as $T_{\mathrm{c}}(\tau) = 0$ for all $\tau < 0$. Likewise, the family of operators $(T_{\mathrm{a}}(\tau))_{\tau \in \mathbb{R}}$ is called an *anti-causal operator*, as $T_{\mathrm{a}}(\tau) = 0$ for all $\tau > 0$. We recall in this section the basic properties of causal and anti-causal operators.

2.3.1 Causal operators

Causal functions have very nice properties, because their Fourier transforms have analytic extensions in the upper half-plane

$$\mathbb{U} := \{z \in \mathbb{C} \mid \operatorname{Im} z > 0\}.$$

This comes from the fact that, if $f \in L^1(\mathbb{R}_\tau) + L^\infty(\mathbb{R}_\tau)$ is such that $f(\tau) = 0$ for $\tau < 0$, the Laplace transform $\widetilde{f}$ of f, defined on $\mathbb{U}$ by[2]

$$\forall z \in \mathbb{U}, \qquad \widetilde{f}(z) := \int_{\mathbb{R}} f(\tau)\mathrm{e}^{\mathrm{i}z\tau}\,\mathrm{d}\tau = \int_0^{+\infty} f(\tau)\mathrm{e}^{\mathrm{i}z\tau}\,\mathrm{d}\tau, \tag{9}$$

is a natural analytic lifting onto $\mathbb{U}$ of the time-Fourier transform $\widehat{f}$ of f defined on $\mathbb{R}_\omega = \partial\mathbb{U}$. Note that the Laplace transform can be extended to appropriate classes of tempered distributions, see [38, Chapter VIII].

Let us first recall the Titchmarsh's theorem [44] (see for instance [30, Section 1.6]).

Theorem 9 (Titchmarsh's theorem in L^2 [44]). *Let $f \in L^2(\mathbb{R}_\tau)$ and $\widehat{f} \in L^2(\mathbb{R}_\omega)$ be its time-Fourier transform. The following assertions are equivalent:*

(i) f is causal (i.e. $f(\tau) = 0$ for almost all $\tau < 0$);

(ii) there exists an analytic function F in the upper half-plane $\mathbb{U}$ satisfying

$$\sup_{\eta > 0} \left(\int_{-\infty}^{+\infty} |F(\omega + \mathrm{i}\eta)|^2 \, \mathrm{d}\omega \right) < \infty$$

and such that, $F(\cdot + \mathrm{i}\eta) \to \widehat{f}$ strongly in $L^2(\mathbb{R}_\omega)$, as $\eta \to 0^+$;

(iii) $\operatorname{Re} \widehat{f}$ and $\operatorname{Im} \widehat{f}$ satisfy the first Plemelj formula

$$\operatorname{Re} \widehat{f} = -\mathfrak{H}\left(\operatorname{Im} \widehat{f} \right) \quad \text{in } L^2(\mathbb{R}_\omega); \tag{10}$$

(iv) $\operatorname{Re} \widehat{f}$ and $\operatorname{Im} \widehat{f}$ satisfy the second Plemelj formula

$$\operatorname{Im} \widehat{f} = \mathfrak{H}\left(\operatorname{Re} \widehat{f} \right) \quad \text{in } L^2(\mathbb{R}_\omega). \tag{11}$$

If these four assertions are satisfied, then the function F in (ii) is unique, and coincides with the Laplace transform $\widetilde{f}$ of f.

We refer to [44] for a proof of this theorem. Formulae (10)-(11) are sometimes referred to as the Kramers-Krönig formulae or the dispersion relations in the physics literature. Titchmarsh's theorem implies in particular that square integrable causal functions, which can be very easily characterized in the time domain (they vanish for negative times), can also be easily characterized in the frequency domain (the imaginary parts of their Fourier transforms are the Hilbert transforms of their real parts).

We emphasize that the above version of Titchmarsh's theorem is only valid in L^2, while the GW setting mostly involves L^∞ causal functions (see Section 3.2 for instance). Weaker versions of Titchmarsh's theorem are available for wider classes of tempered distributions (see [30] and references therein), but the L^∞ setting turns out to be sufficient for our purposes and has the advantage of allowing short, self-contained proofs of all statements. Note that the assertions are no longer equivalent.

---

[2]The Laplace transform is usually defined as

$$F(p) = \int_0^\infty f(\tau)\mathrm{e}^{-p\tau}\,\mathrm{d}\tau.$$

Our definition, which is better adapted to the GW framework, simply amounts to rotating the axis, or, in other words, to setting $z = \mathrm{i}p$.

Theorem 10 (Titchmarsh's theorem in $L^\infty(\mathbb{R})$). *Let $g \in L^\infty(\mathbb{R}_\tau)$ be a causal function (i.e. $g(\tau) = 0$ for $\tau < 0$) and let $\widehat{g} \in H^{-s}(\mathbb{R}_\omega)$ for all $s > 1/2$ be its time-Fourier transform, and $\widetilde{g}$ be its Laplace transform defined on $\mathbb{U}$. Then,*

(i) $\widetilde{g}$ is analytic on $\mathbb{U}$;

(ii) the function $\eta \mapsto \widetilde{g}(\cdot + \mathrm{i}\eta)$ is continuous from $(0, +\infty)$ to $H^s(\mathbb{R}_\omega)$ for all $s \in \mathbb{R}$, and is uniformly continuous from $[0, +\infty)$ to $H^{-s}(\mathbb{R}_\omega)$ for all $s > 1/2$. Moreover, $\widetilde{g}(\cdot + \mathrm{i}\eta) \to \widehat{g}$ strongly in $H^{-s}(\mathbb{R}_\omega)$ for all $s > 1/2$, as $\eta \to 0^+$;

(iii) for all $z \in \mathbb{U}$,

$$\widetilde{g}(z) = \frac{1}{2\mathrm{i}\pi} \left\langle \widehat{g}, (\cdot - z)^{-1} \right\rangle_{H^{-1}, H^1}. \tag{12}$$

(iv) $\operatorname{Re}\widehat{g}$ and $\operatorname{Im}\widehat{g}$ satisfy the Plemelj formulae:

$$\operatorname{Re}\widehat{g} = -\mathfrak{H}\left(\operatorname{Im}\widehat{g}\right) \quad \text{and} \quad \operatorname{Im}\widehat{g} = \mathfrak{H}\left(\operatorname{Re}\widehat{g}\right) \quad \text{in } H^{-1}(\mathbb{R}_\omega). \tag{13}$$

The proof of Theorem 10, which is a simplified version of the proof of the more general result given by [43, Lemma 1] (see also [30, Section 1.7]), is given in Section 6.2. For simplicity, we stated (12) and (13) in H^{-s} for the value $s = 1$, but similar results hold for any value $s > 1/2$.

Let us now extend these results to operator-valued functions. We recall that a map $\widetilde{A}(z)$ from an open set $U \subset \mathbb{C}$ to a Banach space E is said to be strongly analytic on U if $U \ni z \mapsto \widetilde{A}(z) \in E$ is $\mathbb{C}$-differentiable on U, i.e. $\mathrm{d}\widetilde{A}(z)/\mathrm{d}z \in E$ for all $z \in U$.

Definition 11 (bounded causal operator). *Let $\mathcal{H}$ be a Hilbert space and $T_\mathrm{c} \in L^\infty(\mathbb{R}_\tau, \mathcal{B}(\mathcal{H}))$. We say that T_c is a bounded causal operator on $\mathcal{H}$ if $T_\mathrm{c}(\tau) = 0$ for almost all $\tau < 0$.*

Lemma 3 and Theorem 10 can be straightforwardly extended to operator-valued maps (see Section 6.3 for the proof).

Proposition 12. *Let $\mathcal{H}$ be a Hilbert space and $T_\mathrm{c} \in L^\infty(\mathbb{R}_\tau, \mathcal{B}(\mathcal{H}))$ a bounded causal operator on $\mathcal{H}$. Then its time-Fourier transform $\widehat{T}_\mathrm{c}$ belongs to $H^{-s}(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}))$ for any $s > 1/2$, and its Laplace transform*

$$\widetilde{T}_\mathrm{c}(z) := \int_\mathbb{R} T_\mathrm{c}(\tau)\,\mathrm{e}^{\mathrm{i}z\tau}\,\mathrm{d}\tau = \int_0^{+\infty} T_\mathrm{c}(\tau)\,\mathrm{e}^{\mathrm{i}z\tau}\,\mathrm{d}\tau$$

is well defined on the upper-half plane $\mathbb{U}$. Moreover,

(i) $\widetilde{T}_\mathrm{c}$ is a strongly analytic function from $\mathbb{U}$ to $\mathcal{B}(\mathcal{H})$;

(ii) the function $\eta \mapsto \widetilde{T}_\mathrm{c}(\cdot + \mathrm{i}\eta)$ is continuous from $(0, +\infty)$ to $H^s(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}))$ for all $s \in \mathbb{R}$, and uniformly continuous from $[0, +\infty)$ to $H^{-s}(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}))$ for $s > 1/2$. Moreover, for any $s > 1/2$, $\widetilde{T}_\mathrm{c}(\cdot + \mathrm{i}\eta) \to \widehat{T}_\mathrm{c}$ strongly in $H^{-s}(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}))$ as $\eta \to 0^+$;

(iii) for all $z \in \mathbb{U}$, it holds

$$\widetilde{T}_\mathrm{c}(z) = \frac{1}{2\mathrm{i}\pi} \left\langle \widehat{T}_\mathrm{c}, (\cdot - z)^{-1} \right\rangle_{H^{-1}, H^1};$$

(iv) the operators $\operatorname{Re}\widehat{T}_\mathrm{c}$ and $\operatorname{Im}\widehat{T}_\mathrm{c}$ satisfy the Plemelj formulae:

$$\operatorname{Re}\widehat{T}_\mathrm{c} = -\mathfrak{H}\left(\operatorname{Im}\widehat{T}_\mathrm{c}\right) \quad \text{and} \quad \operatorname{Im}\widehat{T}_\mathrm{c} = \mathfrak{H}\left(\operatorname{Re}\widehat{T}_\mathrm{c}\right) \quad \text{in } H^{-1}(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H})). \tag{14}$$

Besides the general case covered by Proposition 12, the particular case of causal time-propagators is often encountered. Explicit formulae can be provided for the Laplace and Fourier transforms in this case, as made precise in the following result (see Section 6.4 for the proof).

Proposition 13 (Analytic extension of causal time propagators)**.** *Let H be a self-adjoint operator on a Hilbert space $\mathcal{H}$ and $A_c(\tau) := -\mathrm{i}\Theta(\tau)\mathrm{e}^{-\mathrm{i}\tau H}$. The Laplace transform $(\widetilde{A}_c(z))_{z\in\mathbb{U}}$ coincides with the resolvent of H in $\mathbb{U}$:*

$$\widetilde{A}_c(z) = (z - H)^{-1}.$$

Moreover, $\widetilde{A}_c(\cdot + \mathrm{i}\eta)$ converge to $\widehat{A}_c$ in $H^{-1}(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}))$ as $\eta \to 0^+$, and

$$\mathrm{Re}\,\widehat{A}_c = \mathrm{p.v.}\left(\frac{1}{\cdot - H}\right) \quad \text{and} \quad \mathrm{Im}\,\widehat{A}_c = -\pi P^H \quad \text{in } H^{-1}(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H})).$$

Let us conclude this section with a useful result (see Section 6.5 for the proof).

Lemma 14. *Consider a bounded causal operator $T_c \in L^\infty(\mathbb{R}_\tau, \mathcal{B}(\mathcal{H}))$ such that $\mathrm{Supp}(\mathrm{Im}\,\widehat{T}_c) \subset [\omega_0, \infty)$ for some $\omega_0 \in \mathbb{R}$. Then $\mathrm{Im}\,\widehat{T}_c \geqslant 0$ on $\mathbb{R}_\omega$ if and only if $\mathrm{Re}\,\widehat{T}_c \geqslant 0$ on $(-\infty, \omega_0]$.*

2.3.2 Anti-causal operators

Definition 15 (bounded anti-causal operator)**.** *Let $\mathcal{H}$ be a Hilbert space and $T_a \in L^\infty(\mathbb{R}_\tau, \mathcal{B}(\mathcal{H}))$. We say that T_a is a bounded anti-causal operator if $T_a(\tau) = 0$ for almost all $\tau > 0$.*

All the results for causal operators stated in the previous section can be straightforwardly transposed to anti-causal operators, by remarking that if $(T_a(\tau))_{\tau\in\mathbb{R}}$ is an anti-causal operator, then $(T_a(-\tau))_{t\in\mathbb{R}}$ is a causal operator. We will use in particular the following results, which are the counterparts of Proposition 12, Proposition 13 and Lemma 14.

Proposition 16. *Let $\mathcal{H}$ be a Hilbert space and $T_a \in L^\infty(\mathbb{R}_\tau, \mathcal{B}(\mathcal{H}))$ a bounded anti-causal operator on $\mathcal{H}$. Then its time-Fourier transform $\widehat{T}_a$ belongs to $H^{-s}(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}))$ for any $s > 1/2$, and its Laplace transform $\widetilde{T}_a$ is well defined on the lower half-plane*

$$\mathbb{L} = \{z \in \mathbb{C} \mid \mathrm{Im}\,(z) < 0\}.$$

Moreover,

(i) $\widetilde{T}_a$ is a strongly analytic function from $\mathbb{L}$ to $\mathcal{B}(\mathcal{H})$;

(ii) the function $\eta \mapsto \widetilde{T}_a(\cdot - \mathrm{i}\eta)$ is continuous from $(0, +\infty)$ to $H^s(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}))$ for all $s \in \mathbb{R}$, and uniformly continuous from $[0, +\infty)$ to $H^{-s}(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}))$ for $s > 1/2$. Moreover, for any $s > 1/2$, $\widetilde{T}_a(\cdot - \mathrm{i}\eta) \to \widehat{T}_a$ strongly in $H^{-s}(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}))$ as $\eta \to 0^+$;

(iii) for all $z \in \mathbb{L}$, it holds

$$\widetilde{T}_a(z) = -\frac{1}{2\mathrm{i}\pi}\left\langle \widehat{T}_a, (\cdot - z)^{-1}\right\rangle_{H^{-1}, H^1};$$

(iv) the operators $\mathrm{Re}\,\widehat{T}_a$ and $\mathrm{Im}\,\widehat{T}_a$ satisfy the Plemelj formulae:

$$\mathrm{Re}\,\widehat{T}_a = \mathfrak{H}\left(\mathrm{Im}\,\widehat{T}_a\right) \quad \text{and} \quad \mathrm{Im}\,\widehat{T}_a = -\mathfrak{H}\left(\mathrm{Re}\,\widehat{T}_a\right) \quad \text{in } H^{-1}(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H})). \tag{15}$$

Note that the signs in the Plemelj formulae are different for causal and anti-causal operators (compare (14) and (15)). Also, the Laplace transform is defined in the lower-half plane $\mathbb{L}$ for anti-causal operators, while it is defined in the upper-half plane $\mathbb{U}$ for causal operators. The counterpart of Proposition 13 is the following proposition.

Proposition 17 (Analytic extension of anti-causal time propagators)**.** *Let H be a self-adjoint operator on a Hilbert space $\mathcal{H}$ and $A_a(\tau) := \mathrm{i}\Theta(-\tau)\mathrm{e}^{\mathrm{i}\tau H}$. The Laplace transform $(\widetilde{A}_a(z))_{z\in\mathbb{L}}$ is*

$$\widetilde{A}_a(z) = (z + H)^{-1}.$$

Moreover, $\widetilde{A}_a(\cdot - \mathrm{i}\eta)$ converge to $\widehat{A}_a$ in $H^{-1}(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}))$ as $\eta \to 0^+$, and

$$\mathrm{Re}\,\widehat{A}_a = \mathrm{p.v.}\left(\frac{1}{\cdot + H}\right) \quad \text{and} \quad \mathrm{Im}\,\widehat{A}_a = \pi P^{-H} \quad \text{in } H^{-1}(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H})).$$

Finally, a result similar to Lemma 14 can also be stated.

Lemma 18. *Consider a bounded anti-causal operator $T_a \in L^\infty(\mathbb{R}_\tau, \mathcal{B}(\mathcal{H}))$ such that $\mathrm{Supp}(\mathrm{Im}\,\widehat{T_a}) \subset (-\infty, \omega_0]$ for some $\omega_0 \in \mathbb{R}_\omega$. Then, $\mathrm{Im}\,\widehat{T_a} \geqslant 0$ if and only if $\mathrm{Re}\,\widehat{T_a}(\omega) \geqslant 0$ on $[\omega_0, +\infty)$.*

2.4 Operators defined by kernel products

Two of the fundamental equations in the GW method (see Sections 4.2.1 and 4.3.1) are of the form

$$\mathcal{C}(\mathbf{x}_1, \mathbf{x}_2) = \mathrm{i}\mathcal{A}(\mathbf{x}_1, \mathbf{x}_2)\mathcal{B}(\mathbf{x}_2, \mathbf{x}_1), \tag{16}$$

where $\mathcal{A}(\mathbf{x}, \mathbf{x}')$ and $\mathcal{B}(\mathbf{x}, \mathbf{x}')$ are the kernels of space-time operators invariant by time translations. As the product of the kernels of two operators is not, in general, the kernel of a well-defined operator, we have to clarify the meaning of (16). We first treat the case of time-independent operators in Section 2.4.1, and consider time-dependent operators and their Laplace transforms in a second step (see Section 2.4.3).

2.4.1 Definition of the kernel product

We first consider the special case when the operators in (16) are time-independent. Our aim is to give a meaning to equalities such as

$$C(\mathbf{r}_1, \mathbf{r}_2) := A(\mathbf{r}_1, \mathbf{r}_2)B(\mathbf{r}_2, \mathbf{r}_1), \tag{17}$$

where $A(\mathbf{r}, \mathbf{r}')$ and $B(\mathbf{r}, \mathbf{r}')$ are the kernels of two integral operators A and B on $L^2(\mathbb{R}^3)$. For this purpose, we replace (17) by the formally equivalent definition

$$\begin{aligned}
\forall (f, g) \in L^2(\mathbb{R}^3) \times L^2(\mathbb{R}^3), \qquad \langle f|C|g \rangle &:= \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \overline{f}(\mathbf{r}_1) C(\mathbf{r}_1, \mathbf{r}_2) g(\mathbf{r}_2) \, \mathrm{d}\mathbf{r}_1 \, \mathrm{d}\mathbf{r}_2 \\
&= \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} A(\mathbf{r}_1, \mathbf{r}_2) g(\mathbf{r}_2) B(\mathbf{r}_2, \mathbf{r}_1) \overline{f}(\mathbf{r}_1) \, \mathrm{d}\mathbf{r}_1 \, \mathrm{d}\mathbf{r}_2 \\
&= \mathrm{Tr}_{L^2(\mathbb{R}^3)} \left(AgB\overline{f} \right),
\end{aligned} \tag{18}$$

where the last line involves the operators A and B themselves, and not their kernels ($\overline{f}$ and g are there seen as multiplication operators by the functions $\overline{f}$ and g respectively).

The formal equalities leading to (18) suggest to define the kernel product of two operators A and B (defined on dense subspaces of $L^2(\mathbb{R}^3)$), as the operator on $L^2(\mathbb{R}^3)$ with domain $D \subset L^2(\mathbb{R}^3)$, denoted by $A \odot B$ and characterized by

$$\forall (f, g) \in L^2(\mathbb{R}^3) \times D, \qquad \langle f|(A \odot B)|g \rangle := \mathrm{Tr}_{L^2(\mathbb{R}^3)} \left(AgB\overline{f} \right). \tag{19}$$

In particular, the product $A \odot B$ is a well-defined bounded operator on $L^2(\mathbb{R}^3)$ as soon as $AgB\overline{f}$ is trace-class for all $(f, g) \in L^2(\mathbb{R}^3) \times L^2(\mathbb{R}^3)$ and $(f, g) \mapsto \mathrm{Tr}_{L^2(\mathbb{R}^3)}(AgB\overline{f})$ is a continuous sesquilinear form on $L^2(\mathbb{R}^3) \times L^2(\mathbb{R}^3)$. It follows from the above considerations that if A and B are operators with well-behaved (for instance smooth and compactly supported) kernels $A(\mathbf{r}_1, \mathbf{r}_2)$ and $B(\mathbf{r}_1, \mathbf{r}_2)$, then $A \odot B$ is a bounded integral operator with kernel $(A \odot B)(\mathbf{r}_1, \mathbf{r}_2) = A(\mathbf{r}_1, \mathbf{r}_2)B(\mathbf{r}_2, \mathbf{r}_1)$.

Remark 19. *It is also possible to rely on the formal equality*

$$\forall (f, g) \in L^2(\mathbb{R}^3) \times L^2(\mathbb{R}^3), \quad \langle f|C|g \rangle = \mathrm{Tr}_{L^2(\mathbb{R}^3)} \left(\overline{f} AgB \right),$$

and define another kernel product $\widetilde{\odot}$ by

$$\forall (f, g) \in L^2(\mathbb{R}^3) \times D, \qquad \left\langle f \left| A \,\widetilde{\odot}\, B \right| g \right\rangle := \mathrm{Tr}_{L^2(\mathbb{R}^3)} \left(\overline{f} AgB \right).$$

It may hold that $A \odot B$ is a well-defined bounded operator, while $A \widetilde{\odot} B$ is an unbounded operator.[3] *In the sequel, we will mostly state the results for the $\odot$ kernel product.*

Remark 20. *The product $A \odot B$ can be seen as an infinite-dimensional extension of the Hadamard product $\mathbf{A} \circ \mathbf{B}^T$ defined for two matrices $\mathbf{A} \in \mathbb{C}^{m \times n}$ and $\mathbf{B} \in \mathbb{C}^{n \times m}$ by*

$$\forall 1 \leqslant i \leqslant m, \quad \forall 1 \leqslant j \leqslant n, \quad \left(\mathbf{A} \circ \mathbf{B}^T \right)_{ij} = \mathbf{A}_{ij} \left(\mathbf{B}^T \right)_{ij} = \mathbf{A}_{ij} \mathbf{B}_{ji}.$$

Let us specify possible sufficient conditions for the operator $A \odot B$ to be well-defined. The typical situation we will encounter in the GW setting (see Sections 4.2.1 and 4.3.1) is the case when $A \in \mathcal{B}(L^2(\mathbb{R}^3))$, while B is an operator on $L^2(\mathbb{R}^3)$ satisfying

$$\forall f, g \in L^2(\mathbb{R}^3), \quad \mathrm{Tr}\left(|gB\overline{f}| \right) \leqslant C_B \|f\|_{L^2} \|g\|_{L^2}. \tag{20}$$

In this case, the operator $A \odot B$ defined in (19) is a well-defined bounded linear operator on $L^2(\mathbb{R}^3)$, and

$$\|A \odot B\|_{\mathcal{B}(L^2(\mathbb{R}^3))} \leqslant C_B \|A\|_{\mathcal{B}(L^2(\mathbb{R}^3))}.$$

The operators B arising in the GW formalism are usually of the form $B = B_1^* B_2 B_1$, where B_1 is an operator from $L^2(\mathbb{R}^3)$ to some Hilbert space $\mathcal{H}$, and $B_2 \in \mathcal{B}(\mathcal{H})$. In fact, assume that the operator B_1 is such that $B_1 f \in \mathfrak{S}_2(L^2(\mathbb{R}^3), \mathcal{H})$ for any $f \in L^2(\mathbb{R}^3)$, with

$$\|B_1 f\|_{\mathfrak{S}_2(L^2(\mathbb{R}^3), \mathcal{H})} \leqslant K \|f\|_{L^2}, \tag{21}$$

for a constant $K \in \mathbb{R}^+$ independent of f. In the left-hand side of (21), f denotes the multiplication operator by the function f. In this case, (20) holds with

$$C_B = K^2 \|B_2\|_{\mathcal{B}(\mathcal{H})}.$$

Let us conclude by giving a simple example when (21) is satisfied, in the situation when $\mathcal{H} = L^2(\mathbb{R}^3)$.

Lemma 21. *Let B_1 be a linear operator with integral kernel $B_1(\mathbf{r}, \mathbf{r}') \in L^2_{\mathrm{loc}}(\mathbb{R}^3 \times \mathbb{R}^3)$, such that $\mathbf{r} \mapsto \|B_1(\mathbf{r}, \cdot)\|_{L^\infty} \in L^2(\mathbb{R}^3)$. Then $B_1 \in \mathcal{B}(L^1(\mathbb{R}^3), L^2(\mathbb{R}^3))$, so that B_1 defines an operator on $L^2(\mathbb{R}^3)$ with domain $L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$. Moreover, for any $f \in L^2(\mathbb{R}^3)$, the operator $B_1 f$ is Hilbert-Schmidt on $L^2(\mathbb{R}^3)$, with*

$$\|B_1 f\|_{\mathfrak{S}_2(L^2(\mathbb{R}^3))} \leqslant \left(\int_{\mathbb{R}^3} \|B_1(\mathbf{r}, \cdot)\|^2_{L^\infty(\mathbb{R}^3)} \, \mathrm{d}\mathbf{r} \right)^{1/2} \|f\|_{L^2(\mathbb{R}^3)}.$$

The proof of this result can be read in Section 6.6. In the GW setting, a technical result similar to Lemma 21 is provided by Lemma 77.

2.4.2 Properties of the kernel product

Lemma 22. *Consider two bounded operators $A, B \in \mathcal{B}(L^2(\mathbb{R}^3))$ such that $A, B \geqslant 0$ and (20) holds. Then, $A \odot B$ is a bounded, positive operator on $L^2(\mathbb{R}^3)$.*

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[3] As an example of such a situation, take $\phi \in L^2(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, $\psi \in L^2(\mathbb{R}^3) \setminus L^\infty(\mathbb{R}^3)$, and set $A = |\psi\rangle\langle\phi|$ and $B = |\phi\rangle\langle\phi|$. Then, for all $f, g \in L^2(\mathbb{R}^3)$, the operator $AgB\overline{f} = |\psi\rangle\langle\phi|g|\phi\rangle\langle\phi f|$ is a well-defined rank-1 bounded operator since $\phi f \in L^2(\mathbb{R}^3)$, hence is trace class. Moreover,

$$\mathrm{Tr}_{L^2(\mathbb{R}^3)}\left(AgB\overline{f} \right) \leqslant \left(\|\phi\|^2_{L^\infty} \|\phi\|_{L^2} \|\psi\|_{L^2} \right) \|f\|_{L^2} \|g\|_{L^2},$$

so that $A \odot B$ is a well-defined bounded operator on $L^2(\mathbb{R}^3)$. On the other hand, it formally holds $\overline{f}AgB = |f\psi\rangle\langle\phi|g|\phi\rangle\langle\phi|$. If f is such that $f\psi \notin L^2(\mathbb{R}^3)$, then this operator is not bounded.
We are grateful to Yanqi Qiu for pointing out this counter-example to our attention.

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The proof of this result is very simple: it relies on the observation that, for any $f \in L^2(\mathbb{R}^3)$,

$$\langle f \,|A \odot B|\, f \rangle = \mathrm{Tr}_{L^2(\mathbb{R}^3)} \left(Af B\overline{f} \right) = \mathrm{Tr}_{L^2(\mathbb{R}^3)} \left(A^{1/2} f B \overline{f} A^{1/2} \right) \geqslant 0,$$

since $fB\overline{f}$ is a positive, trace class operator and $A^{1/2} \geqslant 0$ is a bounded operator.

Lemma 23. *Consider two bounded operators $A, B \in \mathcal{B}(L^2(\mathbb{R}^3))$ such that (20) holds. Then, $A \odot B$ is a bounded operator with adjoint $(A \odot B)^* = A^* \odot B^*$.*

The proof of this result is also elementary: for any $f, g \in L^2(\mathbb{R}^3)$,

$$\langle f \,|\, (A \odot B)\, g \rangle = \mathrm{Tr}_{L^2(\mathbb{R}^3)} \left(Ag B\overline{f} \right) = \overline{\mathrm{Tr}_{L^2(\mathbb{R}^3)} \left(\left(AgB\overline{f} \right)^* \right)} = \overline{\mathrm{Tr}_{L^2(\mathbb{R}^3)} \left(fB^* \overline{g} A^* \right)}$$
$$= \overline{\mathrm{Tr}_{L^2(\mathbb{R}^3)} \left(A^* f B^* \overline{g} \right)} = \overline{\langle g, (A^* \odot B^*) f \rangle} = \langle (A^* \odot B^*) f, g \rangle .$$

In particular, $A \odot B$ is self-adjoint whenever A and B are self-adjoint.

2.4.3 Laplace transforms of kernel products

We finally combine the results on causal operators with those on the kernel product $\odot$ defined in Section 2.4.1 in order to give a meaning to (16). Note first that the space-time operator with kernel $\mathcal{C}(\mathbf{x}, \mathbf{x}')$ is also time-translation invariant and that the family of operators $(A(\tau))_{\tau \in \mathbb{R}}$, $(B(\tau))_{\tau \in \mathbb{R}}$ and $(C(\tau))_{\tau \in \mathbb{R}}$ such that, formally, $\mathcal{A}(\mathbf{x}_1, \mathbf{x}_2) = A(\mathbf{r}_1, \mathbf{r}_2, t_1 - t_2)$, $\mathcal{B}(\mathbf{x}_1, \mathbf{x}_2) = B(\mathbf{r}_1, \mathbf{r}_2, t_1 - t_2)$, and $\mathcal{C}(\mathbf{x}_1, \mathbf{x}_2) = C(\mathbf{r}_1, \mathbf{r}_2, t_1 - t_2)$, are related by

$$C(\tau) = \mathrm{i}A(\tau) \odot B(-\tau). \tag{22}$$

We assume here that A and B are such that (22) is well-defined. When all the operator-valued functions have sufficient regularity in time, their Fourier transforms decay sufficiently fast at infinity and it is possible to Fourier transform (22). This is however not the typical case in the GW setting since we work with causal and anti-causal operators, whose Fourier transforms are in $H^{-s}(\mathbb{R}_\omega)$ for some $s > 1/2$.

We therefore rather consider Laplace transforms. More precisely, for two fields of uniformly bounded operators $(A(\tau))_{\tau \in \mathbb{R}}$ and $(B(\tau))_{\tau \in \mathbb{R}}$, and provided $C(\tau) := \mathrm{i}A(\tau) \odot B(-\tau)$ is well defined, we can decompose A, B and C as the sums of their causal and anti-causal parts as

$$A(\tau) = A^+(\tau) + A^-(\tau) \quad \text{with} \quad A^+(\tau) := \Theta(\tau) A(\tau) \quad \text{and} \quad A^-(\tau) := \Theta(-\tau) A(\tau),$$

and similarly for B and C. Then,

$$C^+(\tau) = \mathrm{i}A^+(\tau) \odot B^-(-\tau) \quad \text{and} \quad C^-(\tau) = \mathrm{i}A^-(\tau) \odot B^+(-\tau). \tag{23}$$

We next consider $\omega > 0$ and $0 < \eta < \omega$. From the equality

$$C^+(\tau) \, \mathrm{e}^{-\omega\tau} = \mathrm{i} \left[A^+(\tau) \, \mathrm{e}^{-(\omega-\eta)\tau} \right] \odot \left[B^-(-\tau) \, \mathrm{e}^{-\eta\tau} \right],$$

we deduce, by Fourier transform, that

$$\widetilde{C^+}(\nu + \mathrm{i}\omega) = \frac{\mathrm{i}}{2\pi} \int_{-\infty}^{+\infty} \widetilde{A^+}\left(\nu - \omega' + \mathrm{i}(\omega - \eta) \right) \odot \widetilde{B^-}(-\omega' - \mathrm{i}\eta) \, \mathrm{d}\omega'. \tag{24}$$

The convolution on the right-hand side is well defined in view of Propositions 12 and 16. It however becomes ill-defined as $\omega, \eta \to 0$. In the case when the causal and anti-causal operators A^+ and B^- under consideration are time-propagators, it is possible to remove this singularity by rewriting the convolution on appropriately shifted imaginary axes.

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Theorem 24. *Consider three Hilbert spaces $\mathcal{H}, \mathcal{H}_a, \mathcal{H}_b$, and assume that*

$$A^+(\tau) = -\mathrm{i}\Theta(\tau)A_1^* \mathrm{e}^{-\mathrm{i}\tau A_2} A_1, \qquad A^-(\tau) = \mathrm{i}\Theta(-\tau)A_1^* \mathrm{e}^{\mathrm{i}\tau A_2} A_1,$$
$$B^+(\tau) = -\mathrm{i}\Theta(\tau)B_1^* \mathrm{e}^{-\mathrm{i}\tau B_2} B_1, \qquad B^-(\tau) = \mathrm{i}\Theta(-\tau)B_1^* \mathrm{e}^{\mathrm{i}\tau B_2} B_1,$$

where $A_1 \in \mathcal{B}(\mathcal{H}, \mathcal{H}_a)$, $B_1 \in \mathcal{B}(\mathcal{H}, \mathcal{H}_b)$ and A_2, B_2 are possibly unbounded, self-adjoint operators on $\mathcal{H}_a$ and $\mathcal{H}_b$ respectively, for which there exist real numbers a, b such that $A_2 \geqslant a$ and $B_2 \geqslant b$. We assume in addition that, for any $f \in \mathcal{H}$, $B_1 f \in \mathfrak{S}_2(\mathcal{H}, \mathcal{H}_b)$ with $\|B_1 f\|_{\mathfrak{S}_2(\mathcal{H}, \mathcal{H}_b)} \leqslant K\|f\|_{\mathcal{H}}$, for a constant $K \in \mathbb{R}^+$ independent of f. Then, the operators C, C^+ and C^- in (22)-(23) are well-defined, the Laplace transforms of C^+ and C^- admit analytical continuations on $\mathbb{U} \cup \mathbb{L} \cup (-\infty, a+b)$ and $\mathbb{U} \cup \mathbb{L} \cup (-(a+b), \infty)$ respectively, and it holds for any $\nu < a + b$ and $\nu' \in (-b, a - \nu)$,

$$\forall \omega \in \mathbb{R}, \qquad \widetilde{C^+}(\nu + \mathrm{i}\omega) = -\frac{1}{2\pi} \int_{-\infty}^{+\infty} \widetilde{A^+}\big(\nu + \nu' + \mathrm{i}(\omega + \omega')\big) \odot \widetilde{B^-}(\nu' + \mathrm{i}\omega') \, \mathrm{d}\omega', \qquad (25)$$

while, for any $\nu > -(a+b)$ and $\nu' \in (-a - \nu, b)$,

$$\forall \omega \in \mathbb{R}, \qquad \widetilde{C^-}(\nu + \mathrm{i}\omega) = -\frac{1}{2\pi} \int_{-\infty}^{+\infty} \widetilde{A^-}\big(\nu + \nu' + \mathrm{i}(\omega + \omega')\big) \odot \widetilde{B^+}(\nu' + \mathrm{i}\omega') \, \mathrm{d}\omega'. \qquad (26)$$

Finally, the following equality holds provided $b > 0$ and $a + b > 0$: for any $\nu \in (-(a+b), a+b)$ and $\nu' \in (-b, b)$,

$$\forall \omega \in \mathbb{R}, \qquad \widetilde{C}(\nu + \mathrm{i}\omega) = -\frac{1}{2\pi} \int_{-\infty}^{+\infty} \widetilde{A}\big(\nu + \nu' + \mathrm{i}(\omega + \omega')\big) \odot \widetilde{B}(\nu' + \mathrm{i}\omega') \, \mathrm{d}\omega'. \qquad (27)$$

The proof of Theorem 24 can be read in Section 6.7. The choices of ν, ν' ensure that the function $\omega' \mapsto \widetilde{A^+}\big(\nu + \nu' + \mathrm{i}(\omega + \omega')\big)$ is in $L^p(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}))$ for any $p > 1$, while, for any $f, g \in \mathcal{H}$, the function $\omega' \mapsto g\widetilde{B^-}(\nu' + \mathrm{i}\omega')\overline{f}$ is in $L^p(\mathbb{R}_\omega, \mathfrak{S}_1(\mathcal{H}))$ for any $p > 1$. Therefore, in view of (25), the function $\omega \mapsto \widetilde{C^+}(\nu + \mathrm{i}\omega)$ is in $L^p(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}))$ for any $p > 1$. Similar results hold for $\omega \mapsto \widetilde{C^-}(\nu + \mathrm{i}\omega)$ and $\omega \mapsto \widetilde{C}(\nu + \mathrm{i}\omega)$.

Let us conclude this section by deducing interesting properties from the analytic continuation results given by Theorem 24 (see Section 6.8 for the proof).

Corollary 25. *Assume that the conditions of Theorem 24 hold. Then,*

$$\mathrm{Supp}\left(\mathrm{Im}\,\widehat{C^+}\right) \subset [a+b, +\infty), \qquad \mathrm{Im}\,\widehat{C^+} \geqslant 0,$$
$$\mathrm{Supp}\left(\mathrm{Im}\,\widehat{C^-}\right) \subset (-\infty, -(a+b)], \qquad \mathrm{Im}\,\widehat{C^-} \geqslant 0, \qquad (28)$$

so that

$$\mathrm{Supp}\left(\mathrm{Im}\,\widehat{C}\right) \subset \mathbb{R} \backslash (-(a+b), a+b), \qquad \mathrm{Im}\,\widehat{C} \geqslant 0.$$

Moreover,

$$\widehat{C^+} = \mathrm{Re}\,\widehat{C^+} \geqslant 0 \quad on \quad \big(-\infty, a+b\big),$$
$$\widehat{C^-} = \mathrm{Re}\,\widehat{C^-} \geqslant 0 \quad on \quad \big(-(a+b), +\infty\big). \qquad (29)$$

In particular, $\widehat{C} = \mathrm{Re}\,\widehat{C} \geqslant 0$ on $\big(-(a+b), a+b\big)$.

2.5 Second quantization formalism

We recall here the definitions of the main mathematical objects used in the second quantization formalism, which are used to define – at least formally – the kernels of the operators arising in the GW method. More details about the second quantization formalism can be found *e.g.* in [9].

We consider a system of N electrons in Coulomb interaction subjected to a time-independent real-valued external potential $v_{\text{ext}} \in L^2(\mathbb{R}^3, \mathbb{R}) + L^\infty(\mathbb{R}^3, \mathbb{R})$. In order to study the response of the system when electrons are added or removed, we embed this N-body problem in a more general framework where the number of electrons is not prescribed. We denote by $\mathcal{H}_1 = L^2(\mathbb{R}^3, \mathbb{C})$ the one-electron state space (the spin variable is omitted for simplicity), by $\mathcal{H}_N = \bigwedge^N \mathcal{H}_1$ the N-electron state space, and by $\mathbb{F} = \oplus_{N=0}^{+\infty} \mathcal{H}_N$ the Fock space, with the convention that $\mathcal{H}_0 = \mathbb{C}$. The Hamiltonian of the N-particle system reads

$$H_N = -\frac{1}{2} \sum_{i=1}^{N} \Delta_{\mathbf{r}_i} + \sum_{i=1}^{N} v_{\text{ext}}(\mathbf{r}_i) + \sum_{1 \leqslant i < j \leqslant N} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}, \qquad (30)$$

and the corresponding Hamiltonian acting on the Fock space is denoted by $\mathbb{H}$, so that $H_N = \mathbb{H}|_{\mathcal{H}_N}$.

For $f \in \mathcal{H}_1$, the creation and annihilation operators $a^\dagger(f)$ and $a(f)$ are the bounded operators on the Fock space $\mathbb{F}$ defined by

$$\forall N \in \mathbb{N}, \quad a^\dagger(f)|_{\mathcal{H}_N} \in \mathcal{B}(\mathcal{H}_N, \mathcal{H}_{N+1}), \qquad a(f)|_{\mathcal{H}_{N+1}} \in \mathcal{B}(\mathcal{H}_{N+1}, \mathcal{H}_N),$$

and for all $\Phi_N \in \mathcal{H}_N$,

$$[a^\dagger(f)\Phi_N](\mathbf{r}_1, \ldots \mathbf{r}_{N+1}) := \frac{1}{\sqrt{N+1}} \sum_{j=1}^{N+1} (-1)^{j+1} f(\mathbf{r}_j) \Phi_N(\mathbf{r}_1, \ldots, \mathbf{r}_{j-1}, \mathbf{r}_{j+1}, \ldots, \mathbf{r}_{N+1}),$$

$$[a(f)\Phi_N](\mathbf{r}_1, \ldots \mathbf{r}_{N-1}) := \sqrt{N} \int_{\mathbb{R}^3} \overline{f}(\mathbf{r}) \Phi_N(\mathbf{r}, \mathbf{r}_1, \ldots, \mathbf{r}_{N-1}) \, d\mathbf{r}. \qquad (31)$$

The creation and annihilation operators satisfy $a^\dagger(f) = a(f)^*$ and the anticommutation relations

$$\forall (f, g) \in \mathcal{H}_1 \times \mathcal{H}_1, \quad [a(f), a(g)]_+ = 0, \quad [a^\dagger(f), a^\dagger(g)]_+ = 0, \quad [a(f), a^\dagger(g)]_+ = \langle f|g \rangle \mathbb{1}_{\mathbb{F}}, \quad (32)$$

where $[A, B]_+ = AB + BA$ is the anti-commutator of the operators A and B, and where $\mathbb{1}_{\mathbb{F}}$ is the identity operator on $\mathbb{F}$. In particular,

$$a^\dagger(f)a(f) + a(f)a^\dagger(f) = \|f\|_{\mathcal{H}_1}^2 \, \mathbb{1}_{\mathbb{F}}.$$

The mappings $\mathcal{H}_1 \ni f \mapsto a^\dagger(f) \in \mathcal{B}(\mathbb{F})$ and $\mathcal{H}_1 \ni f \mapsto a(f) \in \mathcal{B}(\mathbb{F})$ are respectively linear and antilinear.

In most physics articles and textbooks, the GW formalism is presented in terms of the quantum field operators in the position representation $\Psi(\mathbf{r})$ and $\Psi^\dagger(\mathbf{r})$. We recall that, formally,

$$\forall \mathbf{r} \in \mathbb{R}^3, \ \Psi^\dagger(\mathbf{r}) = \sum_{i=1}^{\infty} \overline{\phi_i(\mathbf{r})} a^\dagger(\phi_i), \qquad \Psi(\mathbf{r}) = \sum_{i=1}^{\infty} \phi_i(\mathbf{r}) a(\phi_i),$$

where $\{\phi_i\}_{i \in \mathbb{N}}$ is any orthonormal basis of $\mathcal{H}_1$. Note that for any $f \in \mathcal{H}_1$,

$$\int_{\mathbb{R}^3} \Psi^\dagger(\mathbf{r}) f(\mathbf{r}) d\mathbf{r} = a^\dagger(f) \quad \text{and} \quad \int_{\mathbb{R}^3} \Psi(\mathbf{r}) f(\mathbf{r}) d\mathbf{r} = a(\overline{f}).$$

In the second-quantization formalism, $\mathbb{H}$ reads,

$$\mathbb{H} = \int_{\mathbb{R}^3} \Psi^\dagger(\mathbf{r}) \left(-\frac{1}{2} \Delta_{\mathbf{r}} + v_{\text{ext}}(\mathbf{r}) \right) \Psi(\mathbf{r}) \, d\mathbf{r} + \frac{1}{2} \int_{(\mathbb{R}^3)^2} \Psi^\dagger(\mathbf{r}) \Psi^\dagger(\mathbf{r}') |\mathbf{r} - \mathbf{r}'|^{-1} \Psi(\mathbf{r}') \Psi(\mathbf{r}) \, d\mathbf{r} \, d\mathbf{r}'.$$

Finally, we introduce the Heisenberg representation of the annihilation and creation field operators $\Psi_{\text{H}}(\mathbf{r}t)$ and $\Psi_{\text{H}}^\dagger(\mathbf{r}t)$, formally defined by

$$\Psi_{\text{H}}^\dagger(\mathbf{r}t) = e^{it\mathbb{H}} \Psi^\dagger(\mathbf{r}) e^{-it\mathbb{H}} \quad \text{and} \quad \Psi_{\text{H}}(\mathbf{r}t) = e^{it\mathbb{H}} \Psi(\mathbf{r}) e^{-it\mathbb{H}}.$$

Note that, still formally, $\Psi_{\text{H}}(\mathbf{r}t)^* = \Psi_{\text{H}}^\dagger(\mathbf{r}t)$, and

$$\Psi_{\text{H}}^\dagger(\mathbf{r}t)\big|_{\mathcal{H}_N} = e^{itH_{N+1}} \Psi^\dagger(\mathbf{r}) \, e^{-itH_N}, \qquad \Psi_{\text{H}}(\mathbf{r}t)\big|_{\mathcal{H}_{N+1}} = e^{itH_N} \Psi(\mathbf{r}) \, e^{-itH_{N+1}}. \qquad (33)$$

3 Operators arising in the GW method for finite systems

This section aims at providing rigorous mathematical definitions of the operators arising in the GW method. For each one of them, we first recall the formal definition given in the physics literature, using the second quantization formalism. We then explain how to recast this formal definition into a (formally equivalent) satisfactory mathematical definition involving only well-defined operators on the k-particle spaces $\mathcal{H}_k$, with $k = 1, N-1, N, N+1$, the Coulomb space $\mathcal{C}$ (defined in Section 3.3.1), and its dual $\mathcal{C}'$. We finally establish some mathematical properties of the operator under consideration, using our definition as a starting point. Unless otherwise specified, scalar products and norms are by default considered on $\mathcal{H}_1 = L^2(\mathbb{R}^3, \mathbb{C})$.

We first need to make some assumptions on the physical system under consideration (see Section 3.1). We can then define the one-body Green's functions in Section 3.2. Linear response operators are considered in Section 3.3, which culminates with the definition of the dynamically screened interaction operator W. We finally introduce the self-energy operator in Section 3.4.

3.1 Assumptions on the reference N-electron system

Recall that the reference system with N electrons is described by the Hamiltonian H_N on $\mathcal{H}_N$ defined by (30). Our first assumption concerns the ground state energy E_N^0 of the reference system described by H_N:

> **Hyp. 1:** The ground state energy E_N^0 is a simple discrete eigenvalue of H_N.

In this case, the normalized ground state wave-function Ψ_N^0 of the reference system is unique up to a global phase. We also define the energy of the first excited state:

$$E_N^1 = \min\left(\sigma(H_N)\backslash\{E_N^0\}\right).$$

Together with Ψ_N^0, we introduce the ground state one-body reduced density-matrix

$$\gamma_N^0(\mathbf{r}, \mathbf{r}') := N \int_{(\mathbb{R}^3)^{N-1}} \Psi_N^0(\mathbf{r}, \mathbf{r}_2, \cdots, \mathbf{r}_N)\overline{\Psi_N^0(\mathbf{r}', \mathbf{r}_2, \cdots, \mathbf{r}_N)}\, \mathrm{d}\mathbf{r}_2 \cdots \mathrm{d}\mathbf{r}_N, \tag{34}$$

the ground state density

$$\rho_N^0(\mathbf{r}) := \gamma_N^0(\mathbf{r}, \mathbf{r}) = N \int_{(\mathbb{R}^3)^{N-1}} |\Psi_N^0(\mathbf{r}, \mathbf{r}_2, \cdots, \mathbf{r}_N)|^2\, \mathrm{d}\mathbf{r}_2 \cdots \mathrm{d}\mathbf{r}_N,$$

and the ground state two-body density

$$\rho_{N,2}^0(\mathbf{r}, \mathbf{r}') := \frac{N(N-1)}{2} \int_{(\mathbb{R}^3)^{N-2}} |\Psi_N^0(\mathbf{r}, \mathbf{r}', \mathbf{r}_3, \cdots, \mathbf{r}_N)|^2\, \mathrm{d}\mathbf{r}_3 \cdots \mathrm{d}\mathbf{r}_N \tag{35}$$

of the reference N-electron system.

We recall in the following proposition some important properties on Ψ_N^0, γ_N^0, ρ_N^0 and $\rho_{N,2}^0$ (most of the assertions below are well known; we provide elements of proof in Section 6.9 for the less standard statements). Note that both $\gamma_N^0(\mathbf{r}, \mathbf{r}')$ and $\rho_{N,2}^0(\mathbf{r}, \mathbf{r}')$ can be seen as the kernels of bounded operators on $\mathcal{H}_1 = L^2(\mathbb{R}^3)$ that we also denote by γ_N^0 and $\rho_{N,2}^0$.

Proposition 26 (Properties of the ground state)**.** *Assume that v_{ext} is of the form*

$$v_{\mathrm{ext}}(\mathbf{r}) = -\sum_{k=1}^{M} \frac{z_k}{|\mathbf{r} - \mathbf{R}_k|},$$

with $z_k \in \mathbb{N}^*$ and $\mathbf{R}_k \in \mathbb{R}^3$ for all $1 \leqslant k \leqslant M$, and that **Hyp. 1** *is satisfied. Then,*

(1) *the ground state wave-function Ψ_N^0 can be chosen real-valued and $\Psi_N^0 \in H^2(\mathbb{R}^{3N})$;*

(2) *the ground state density ρ_N^0 is in $L^1(\mathbb{R}^3, \mathbb{R}) \cap L^\infty(\mathbb{R}^3, \mathbb{R})$ and $\nabla\sqrt{\rho_N^0} \in \left(L^2(\mathbb{R}^3, \mathbb{R})\right)^3$. Moreover, ρ_N^0 is continuous and everywhere positive on $\mathbb{R}^3$;*

(3) *the ground state one-body reduced density operator γ_N^0 is in*

$$\mathcal{K}_N := \left\{ \gamma_N \in \mathcal{S}(\mathcal{H}_1) \;\middle|\; 0 \leqslant \gamma_N \leqslant 1,\; \mathrm{Tr}_{\mathcal{H}_1}(\gamma_N) = N,\; \mathrm{Tr}_{\mathcal{H}_1}(|\nabla|\gamma_N|\nabla|) < \infty \right\},$$

and satisfies
$$\forall (f,g) \in \mathcal{H}_1 \times \mathcal{H}_1, \qquad \langle f|\gamma_N^0|g\rangle = \langle \Psi_N^0|a^\dagger(g)a(f)|\Psi_N^0\rangle_{\mathcal{H}_N}; \tag{36}$$

(4) *the kernel $\gamma_N^0(\mathbf{r}, \mathbf{r}')$ satisfies the pointwise estimate $|\gamma_N^0(\mathbf{r}, \mathbf{r}')|^2 \leqslant \rho_N^0(\mathbf{r})\rho_N^0(\mathbf{r}')$;*

(5) *the operator $\rho_{N,2}^0$ belongs to $\mathcal{S}(\mathcal{H}_1)$, and $\|\rho_{N,2}^0\|_{\mathcal{B}(\mathcal{H}_1)} \leqslant \dfrac{N-1}{2}\|\rho_N^0\|_{L^\infty}$.*

Much finer regularity results on Ψ_N^0 are available [13, 14, 48], but are not needed for our purpose. Similar results hold true if v_{ext} is replaced by a potential generated by smeared nuclei or pseudo-potentials.

Our second assumption is concerned with the (discrete) convexity of $N \mapsto E_N^0$. We assume that $N \geqslant 1$, and that (with the convention $E_0^0 = 0$ in the case $N = 1$)

$$\boxed{\textbf{Hyp. 2: } E_N^0 - E_{N-1}^0 < E_{N+1}^0 - E_N^0.}$$

In this case, any real number μ such that $E_N^0 - E_{N-1}^0 < \mu < E_{N+1}^0 - E_N^0$ is an admissible chemical potential (Fermi level) of the electrons for the ground state of the reference system. The physical relevance of this assumption is discussed for instance in [11, Section 4.2].

3.2 Green's functions

We begin our journey in the GW formalism with Green's functions. The GW method has been designed from the equation of motion for the time-ordered one-body Green's function G [18], which is the concatenation of two meaningful physical objects: the particle Green's function G_p and the hole Green's function G_h.

3.2.1 The particle Green's function G_p

Rigorous definition of the particle Green's function. The particle (or forward, or retarded) Green's function is formally defined by (see for instance [12, Section 7])

$$\mathcal{G}_\mathrm{p}(\mathbf{r}t, \mathbf{r}'t') := -\mathrm{i}\Theta(t - t')\,\langle \Psi_N^0|\Psi_\mathrm{H}(\mathbf{r}t)\Psi_\mathrm{H}^\dagger(\mathbf{r}'t')|\Psi_N^0\rangle, \tag{37}$$

where Θ is the Heaviside function (2), and $\Psi_\mathrm{H}(\mathbf{r}t)$ and $\Psi_\mathrm{H}^\dagger(\mathbf{r}t)$ are the Heisenberg representations of the annihilation and creation field operators introduced in Section 2.5. As $\Psi_N^0 \in \mathcal{H}_N$, we can replace $\Psi(\mathbf{r}t)$ and $\Psi^\dagger(\mathbf{r}t)$ by their expressions (33):

$$\mathcal{G}_\mathrm{p}(\mathbf{r}t, \mathbf{r}'t') = -\mathrm{i}\Theta(t - t')\,\langle \Psi_N^0|\mathrm{e}^{\mathrm{i}tH_N}\Psi(\mathbf{r})\mathrm{e}^{-\mathrm{i}(t-t')H_{N+1}}\Psi^\dagger(\mathbf{r}')\mathrm{e}^{-\mathrm{i}t'H_N}|\Psi_N^0\rangle$$
$$= -\mathrm{i}\Theta(t - t')\,\langle \Psi_N^0|\Psi(\mathbf{r})\mathrm{e}^{-\mathrm{i}(t-t')(H_{N+1}-E_N^0)}\Psi^\dagger(\mathbf{r}')|\Psi_N^0\rangle.$$

As $\mathcal{G}_\mathrm{p}$ only depends on the time difference $t - t'$, it is sufficient to study the function $G_\mathrm{p}(\mathbf{r}, \mathbf{r}', \tau) := \mathcal{G}_\mathrm{p}(\mathbf{r}\tau, \mathbf{r}'0)$. We then notice that, for all $f \in \mathcal{H}_1$,

$$\int_{\mathbb{R}^3} \Psi^\dagger(\mathbf{r}')|\Psi_N^0\rangle f(\mathbf{r}')\,\mathrm{d}\mathbf{r}' = a^\dagger(f)|\Psi_N^0\rangle.$$

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Introducing

$$A_+^* : \quad \mathcal{H}_1 \quad \rightarrow \quad \mathcal{H}_{N+1}$$
$$f \quad \mapsto \quad a^\dagger(f)|\Psi_N^0\rangle$$

and $A_+ = (A_+^*)^*$, we observe that $G_{\mathrm{p}}(\mathbf{r}, \mathbf{r}', \tau)$ is formally the kernel of the following one-body operator.

Definition 27 (Particle Green's function). *The particle Green's function is defined as*

$$G_{\mathrm{p}}(\tau) := -\mathrm{i}\Theta(\tau)\, A_+ \mathrm{e}^{-\mathrm{i}\tau(H_{N+1}-E_N^0)} A_+^*. \tag{38}$$

First properties of the particle Green's function. The study of G_{p} can be decomposed into the study of the operators A_+ and $\mathrm{e}^{-\mathrm{i}\tau(H_{N+1}-E_N^0)}$. The latter is clearly bounded on $\mathcal{H}_{N+1}$. As for the operator A_+^*, we deduce from (32) and (36) that

$$\langle a^\dagger(f)\Psi_N^0 | a^\dagger(g)\Psi_N^0 \rangle = \langle \Psi_N^0 | a(f)a^\dagger(g) | \Psi_N^0 \rangle = \langle f|g \rangle - \langle \Psi_N^0 | a^\dagger(g)a(f) | \Psi_N^0 \rangle = \langle f|1 - \gamma_N^0 | g \rangle,$$

or equivalently,

$$A_+ A_+^* = \mathbb{1}_{\mathcal{H}_1} - \gamma_N^0. \tag{39}$$

Hence, A_+^* is a bounded operator from $\mathcal{H}_1$ to $\mathcal{H}_{N+1}$, and A_+ is a bounded operator from $\mathcal{H}_{N+1}$ to $\mathcal{H}_1$. In fact, since

$$\|A_+^* f\|_{\mathcal{H}_{N+1}}^2 = \left\langle f | (\mathbb{1}_{\mathcal{H}_1} - \gamma_N^0) | f \right\rangle = \left\| (\mathbb{1}_{\mathcal{H}_1} - \gamma_N^0) f \right\|_{\mathcal{H}_1}^2,$$

it holds $\|A_+^*\|_{\mathcal{B}(\mathcal{H}_1, \mathcal{H}_{N+1})} = 1$. The following properties are obtained as a direct corollary of Proposition 13.

Proposition 28 (Properties of the particle Green's function). *The family $(G_{\mathrm{p}}(\tau))_{\tau \in \mathbb{R}}$ defines a bounded causal operator on $\mathcal{H}_1$. The real and imaginary parts of its time-Fourier transform are in $H^{-s}(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$ for all $s > 1/2$, and are given by*

$$\mathrm{Re}\,\widehat{G_{\mathrm{p}}} = A_+ \mathrm{p.v.} \left(\frac{1}{\cdot - (H_{N+1}-E_N^0)} \right) A_+^* \quad and \quad \mathrm{Im}\,\widehat{G_{\mathrm{p}}} = -\pi A_+ P^{H_{N+1}-E_N^0} A_+^*. \tag{40}$$

The analytic operator-valued function $\widetilde{G}_{\mathrm{p}}$ defined in the upper half-plane by

$$\forall z \in \mathbb{U}, \quad \widetilde{G}_{\mathrm{p}}(z) := A_+ \frac{1}{z - (H_{N+1}-E_N^0)} A_+^* \tag{41}$$

is the Laplace transform of G_{p} and satisfies

$$\widehat{G_{\mathrm{p}}} = \lim_{\eta \to 0^+} \widetilde{G}_{\mathrm{p}}(. + \mathrm{i}\eta) \quad in \;\; H^{-s}(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1)) \quad for \; all \;\; s > 1/2.$$

The imaginary part of $\widehat{G_{\mathrm{p}}}$ is related to the so-called spectral function $\mathcal{A}_{\mathrm{p}}$ (see Section 3.2.4).

Analytic continuation to the complex plane. Let us introduce the particle optical excitation set

$$S_{\mathrm{p}} := \sigma(H_{N+1} - E_N^0). \tag{42}$$

We recall that the operator $H_{N+1} - E_N^0$ with domain $\mathcal{H}_{N+1} \cap H^2(\mathbb{R}^{3(N+1)})$ is self-adjoint on $\mathcal{H}_{N+1}$. Its essential spectrum is of the form $\sigma_{\mathrm{ess}}(H_{N+1}-E_N^0) = [\Sigma_{N+1}, \infty)$, and there are possibly infinitely many eigenvalues below Σ_{N+1} that can only accumulate at Σ_{N+1}. According to the HVZ theorem [21, 45, 49], $\Sigma_{N+1} = E_N^0 - E_N^0 = 0$. In particular, S_{p} is the union of a discrete negative part, and the half-line $[0, +\infty)$.

We next infer from (41) that $\widetilde{G}_{\mathrm{p}}(z)$ can be extended to an analytic function from $\mathbb{C} \setminus S_{\mathrm{p}}$ to $\mathcal{B}(\mathcal{H}_1)$. This is of particular interest for the following reason. The operator-valued distribution

$\widehat{G_{\mathrm{p}}}(\omega)$ is highly peaked and irregular (for instance, its imaginary part is a sum of Dirac measures on the discrete part of S_{p}). Instead of studying $\widehat{G_{\mathrm{p}}}(\omega)$ on the real axis, we will study its analytic continuation $\widetilde{G_{\mathrm{p}}}(z)$ (defined *a priori* only in the upper-half plane, but actually on $\mathbb{C} \setminus S_{\mathrm{p}}$) *on the imaginary axis* $\mu + \mathrm{i}\mathbb{R}$, where $\mu < E_{N+1}^0 - E_N^0 \leqslant 0$ is an admissible chemical potential (see **Hyp. 2**). The set S_{p} can be recovered from $\omega \mapsto \widetilde{G_{\mathrm{p}}}(\mu + \mathrm{i}\omega)$ by locating the singularities of $\widehat{G_{\mathrm{p}}}$, obtained from $\widetilde{G_{\mathrm{p}}}$ either by analytic continuation, or by fitting some parameters [36]. We do not address this interesting numerical reconstruction problem in the present article.
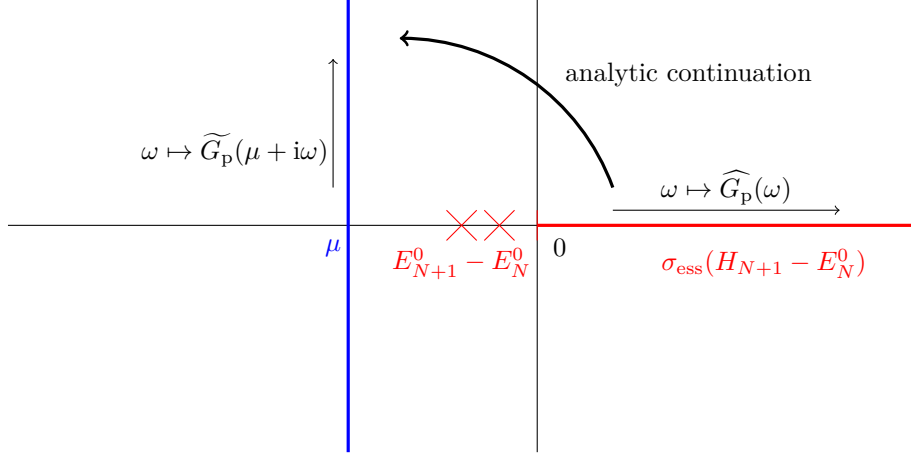

Figure 1: Illustration of the analytic continuation: from $\omega \mapsto \widehat{G_{\mathrm{p}}}(\omega)$ to $\omega \mapsto \widetilde{G_{\mathrm{p}}}(\mu + \mathrm{i}\omega)$.

The following lemma makes precise the behavior of the Green's function on the vertical axis $\mu + \mathrm{i}\mathbb{R}$. It is a direct consequence of the representation (41).

Lemma 29. *Consider $\mu < E_{N+1}^0 - E_N^0$. Then the function $\omega \mapsto \widetilde{G_{\mathrm{p}}}(\mu + \mathrm{i}\omega)$ is real analytic from $\mathbb{R}_\omega$ to $\mathcal{B}(\mathcal{H}_1)$ and is in $L^p(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$ for all $p > 1$. Moreover, for all $\omega \in \mathbb{R}$,*

$$\mathrm{Re}\,\widetilde{G_{\mathrm{p}}}(\mu + \mathrm{i}\omega) = -A_+ \frac{H_{N+1} - E_N^0 - \mu}{\omega^2 + (H_{N+1} - E_N^0 - \mu)^2} A_+^*$$

is a negative, bounded, self-adjoint operator on $\mathcal{H}_1$ which enjoys the following symmetry property:

$$\forall \omega \in \mathbb{R}_\omega, \quad \mathrm{Re}\,\widetilde{G_{\mathrm{p}}}(\mu + \mathrm{i}\omega) = \mathrm{Re}\,\widetilde{G_{\mathrm{p}}}(\mu - \mathrm{i}\omega).$$

For any $f \in \mathcal{H}_1$, the function $\omega \mapsto \langle f | \mathrm{Re}\,\widetilde{G_{\mathrm{p}}}(\mu + \mathrm{i}\omega) | f \rangle$ is non-positive, in $L^1(\mathbb{R}_\omega)$, and

$$\int_{-\infty}^{+\infty} \left\langle f \left| \mathrm{Re}\,\widetilde{G_{\mathrm{p}}}(\mu + \mathrm{i}\omega) \right| f \right\rangle \mathrm{d}\omega = -\pi \langle f | (\mathbb{1}_{\mathcal{H}_1} - \gamma_N^0) | f \rangle. \tag{43}$$

The last assertion comes from the spectral theorem, (39), and the equality

$$\forall E > 0, \qquad \int_{-\infty}^{+\infty} \frac{E}{\omega^2 + E^2}\,\mathrm{d}\omega = \pi.$$

Remark 30. *Unfortunately, although $\mathrm{Re}\,\widetilde{G_{\mathrm{p}}}(\mu + \mathrm{i}\cdot)$ has a sign and (43) is satisfied for all $f \in \mathcal{H}_1$, the function $\omega \mapsto \left\| \mathrm{Re}\,\widetilde{G_{\mathrm{p}}}(\mu + \mathrm{i}\cdot) \right\|_{\mathcal{B}(\mathcal{H}_1)}$ does not belong to $L^1(\mathbb{R}_\omega)$. This is essentially due to the fact that*

$$\sup_{E \geqslant 0} \left(\frac{E}{\omega^2 + E^2} \right) = \frac{1}{2\omega} \notin L^1(\mathbb{R}_\omega).$$

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Note that the imaginary part of $\widetilde{G_{\mathrm{p}}}(\mu + \mathrm{i}\omega)$,

$$\mathrm{Im}\,\widetilde{G_{\mathrm{p}}}(\mu + \mathrm{i}\omega) = -A_+ \frac{\omega}{\omega^2 + (H_{N+1} - E_N^0 - \mu)^2} A_+^*,$$

has no definite sign on $\mathbb{R}_\omega$, and that, for a generic $f \in \mathcal{H}_1$, the function $\omega \mapsto \left\langle f \left| \mathrm{Im}\,\widetilde{G_{\mathrm{p}}}(\mu + \mathrm{i}\omega) \right| f \right\rangle$ does not belong to $L^1(\mathbb{R}_\omega)$. It will therefore be more convenient in general to work with the real part of $\widetilde{G_{\mathrm{p}}}(\mathrm{i}\omega)$ only, especially since the imaginary part can be recovered from the real part (see Lemma 31 below). Indeed, the operator-valued functions $\widetilde{g_{\mathrm{p},\eta}} : \omega \mapsto \widetilde{G_{\mathrm{p}}}(\mu - \eta + \mathrm{i}\omega)$ are in $L^2(\mathbb{R}, \mathcal{B}(\mathcal{H}_1))$ for any $\eta > 0$, and converge to $\widetilde{g_{\mathrm{p}}} : \omega \mapsto \widetilde{G_{\mathrm{p}}}(\mu + \mathrm{i}\omega)$ in $L^2(\mathbb{R}, \mathcal{B}(\mathcal{H}_1))$ as $\eta \to 0^+$. We can therefore apply Titchmarsh's theorem (see Theorem 9), which gives the following result.

Lemma 31. *Let $\mu < E_{N+1}^0 - E_N^0$. The function $\widehat{g_{\mathrm{p}}}(\omega) := \widetilde{G_{\mathrm{p}}}(\mu + \mathrm{i}\omega)$ is the Fourier transform of the causal function*

$$g_{\mathrm{p}}(\tau) = -\Theta(\tau) A_+ \mathrm{e}^{-\tau(H_{N+1} - E_N^0 - \mu)} A_+^*, \tag{44}$$

which belongs to $L^2(\mathbb{R}_\tau, \mathcal{S}(\mathcal{H}_1))$. In particular, the Plemelj formulae hold true:

$$\mathrm{Re}\,\widehat{g_{\mathrm{p}}} = -\mathfrak{H}\left(\mathrm{Im}\,\widehat{g_{\mathrm{p}}}\right) \quad \text{and} \quad \mathrm{Im}\,\widehat{g_{\mathrm{p}}} = \mathfrak{H}\left(\mathrm{Re}\,\widehat{g_{\mathrm{p}}}\right) \quad \text{in } L^2(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1)).$$

Moreover, the function $\tau \mapsto \|g_{\mathrm{p}}(\tau)\|_{\mathcal{B}(\mathcal{H}_1)}$ is exponentially decreasing as $|\tau| \to +\infty$.

Remark 32. *The exponential decay of g_{p} is consistent with the analyticity of its Fourier transform. This property is of interest when calculating numerically convolutions on the imaginary axis $\mu + \mathrm{i}\mathbb{R}$, since convolutions can be replaced, up to a Fourier transform, with point-wise multiplications of causal functions which are exponentially decreasing. This approach was advocated in [34], and is now routinely used in GW computations.*

3.2.2 The hole (backward) Green's function G_{h}

Definition and first properties of the hole Green's function. Together with the particle Green's function, we introduce the hole (or backward, or advanced) Green's function, formally defined within the second quantization formalism by

$$\mathcal{G}_{\mathrm{h}}(\mathbf{r}t, \mathbf{r}'t') := \mathrm{i}\Theta(t' - t)\,\langle \Psi_N^0 | \Psi_{\mathrm{H}}^\dagger(\mathbf{r}'t') \Psi_{\mathrm{H}}(\mathbf{r}t) | \Psi_N^0 \rangle.$$

Observing that

$$\int_{\mathbb{R}^3} \Psi(\mathbf{r}) | \Psi_N^0 \rangle f(\mathbf{r})\,d\mathbf{r} = a(\overline{f}) | \Psi_N^0 \rangle,$$

we introduce

$$\begin{array}{rccc} A_- : & \mathcal{H}_1 & \to & \mathcal{H}_{N-1} \\ & f & \mapsto & a(\overline{f}) | \Psi_N^0 \rangle. \end{array}$$

Similarly as before, we note that $\mathcal{G}_{\mathrm{h}}(\mathbf{r}t, \mathbf{r}'t')$ only depends on the time difference $t - t'$. Introducing $G_{\mathrm{h}}(\mathbf{r}, \mathbf{r}', \tau) := \mathcal{G}_{\mathrm{h}}(\mathbf{r}\tau, \mathbf{r}'0)$, we see that $G_{\mathrm{h}}(\mathbf{r}, \mathbf{r}', \tau)$ is formally the kernel of the following one-body operator.

Definition 33. *The hole Green's function is defined as*

$$G_{\mathrm{h}}(\tau) := \mathrm{i}\Theta(-\tau) A_-^* \mathrm{e}^{\mathrm{i}\tau(H_{N-1} - E_N^0)} A_-. \tag{45}$$

Similarly as in (39), it holds that

$$A_-^* A_- = \gamma_N^0.$$

Hence, A_- is a bounded operator from $\mathcal{H}_1$ to $\mathcal{H}_{N-1}$, A_-^* is a bounded operator from $\mathcal{H}_{N-1}$ to $\mathcal{H}_1$, and it holds $\|A_-\|_{\mathcal{B}(\mathcal{H}_1, \mathcal{H}_N)} = \|A_-^*\|_{\mathcal{B}(\mathcal{H}_{N-1}, \mathcal{H}_1)} \leqslant 1$. The properties of the hole Green's function are quite similar to the properties of the particle Green's function (compare with Proposition 28).

Proposition 34 (Properties of the hole Green's function)**.** *The family* $(G_{\mathrm{h}}(\tau))_{\tau \in \mathbb{R}}$ *defines a bounded anti-causal operator on* $\mathcal{H}_1$*. The real and imaginary parts of its time-Fourier transform are in* $H^{-s}(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$ *for all* $s > 1/2$*, and are given by*

$$\mathrm{Re}\,\widehat{G_{\mathrm{h}}} = A_-^* \,\mathrm{p.v.}\left(\frac{1}{\cdot - (E_N^0 - H_{N-1})}\right) A_- \quad and \quad \mathrm{Im}\,\widehat{G_{\mathrm{h}}} = \pi A_-^* P^{E_N^0 - H_{N-1}} A_-. \tag{46}$$

The analytic operator-valued function $\widetilde{G_{\mathrm{h}}}$ *defined in the lower half-plane by*

$$\forall z \in \mathbb{L}, \qquad \widetilde{G_{\mathrm{h}}}(z) := A_-^* \frac{1}{z - (E_N^0 - H_{N-1})} A_- \tag{47}$$

is the Laplace transform of G_{h} *and satisfies*

$$\widehat{G_{\mathrm{h}}} = \lim_{\eta \to 0^+} \widetilde{G_{\mathrm{h}}}(. - \mathrm{i}\eta) \quad in \ H^{-s}(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H})) \quad for \ all \quad s > 1/2.$$

Analytic continuation into the complex plane. The hole optical excitation set is defined as

$$S_{\mathrm{h}} := \sigma(E_N^0 - H_{N-1}). \tag{48}$$

It is clear from (47) that the operator-valued function $\widetilde{G_{\mathrm{h}}}$ can be analytically continued to $\mathbb{C} \setminus S_{\mathrm{h}}$. Instead of studying the highly irregular distribution $\omega \mapsto \widehat{G_{\mathrm{h}}}(\omega)$, it is more convenient to study its analytical continuation $\widetilde{G_{\mathrm{h}}}$ on the imaginary axis $\mu + \mathrm{i}\mathbb{R}$, with $\mu > E_N^0 - E_{N-1}^0$.
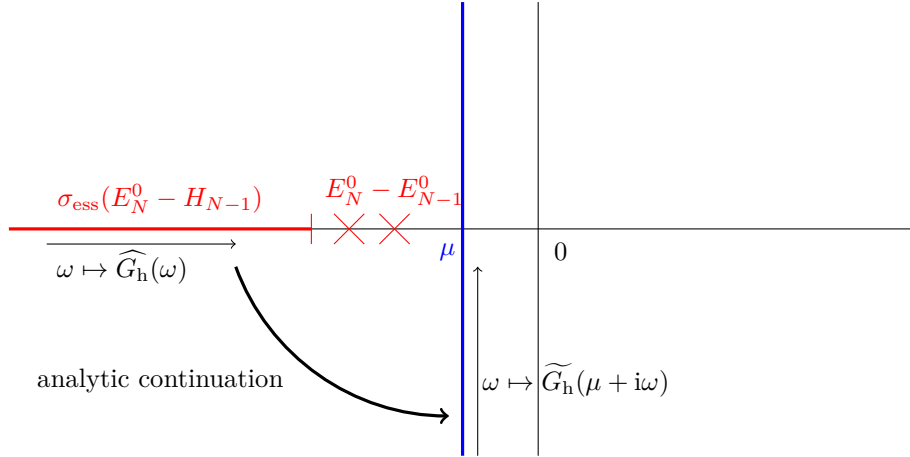
Figure 2: Illustration of the analytic continuation: from $\omega \mapsto \widehat{G_{\mathrm{h}}}(\omega)$ to $\omega \mapsto \widetilde{G_{\mathrm{h}}}(\mu + \mathrm{i}\omega)$.

We can state a result similar to Lemma 29.

Lemma 35. *Consider* $\mu > E_N^0 - E_{N-1}^0$*. Then the function* $\omega \mapsto \widetilde{G_{\mathrm{h}}}(\mu + \mathrm{i}\omega)$ *is real analytic from* $\mathbb{R}_\omega$ *to* $\mathcal{B}(\mathcal{H}_1)$ *and is in* $L^p(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$*, for all* $p > 1$*. Moreover, for all* $\omega \in \mathbb{R}$*,*

$$\mathrm{Re}\,\widetilde{G_{\mathrm{h}}}(\mu + \mathrm{i}\omega) = A_-^* \frac{H_{N-1} + \mu - E_N^0}{\omega^2 + (E_N^0 - H_{N-1} - \mu)^2} A_-$$

is a positive, bounded, self-adjoint operator, which enjoys the following symmetry property:

$$\forall \omega \in \mathbb{R}_\omega, \quad \mathrm{Re}\,\widetilde{G_{\mathrm{h}}}(\mu + \mathrm{i}\omega) = \mathrm{Re}\,\widetilde{G_{\mathrm{h}}}(\mu - \mathrm{i}\omega).$$

For any $f \in \mathcal{H}_1$*, the function* $\omega \mapsto \left\langle f \left| \left| \mathrm{Re}\,\widetilde{G_{\mathrm{h}}}(\mu + \mathrm{i}\omega) \right| \right| f \right\rangle$ *is non-negative, in* $L^1(\mathbb{R}_\omega)$*, and*

$$\int_{-\infty}^{+\infty} \left\langle f \left| \mathrm{Re}\,\widetilde{G_{\mathrm{h}}}(\mu + \mathrm{i}\omega) \right| f \right\rangle \mathrm{d}\omega = \pi \langle f | \gamma_N^0 | f \rangle.$$

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The Galitskii-Migdal formula. The hole Green's function is of particular interest, as it contains useful information on the N-body ground state. For instance, from the identity $A_-^* A_- = \gamma_N^0$, we directly obtain $G_{\mathrm{h}}(0^-) = \mathrm{i}\gamma_N^0$, so that the expectation value in the ground state of any one-body operator $\sum_{i=1}^N C_{\mathbf{r}_i}$ (for $C \in \mathcal{B}(\mathcal{H}_1)$) can be evaluated via

$$\left\langle \Psi_N^0 \left| \sum_{i=1}^N C_{\mathbf{r}_i} \right| \Psi_N^0 \right\rangle = \mathrm{Tr}_{\mathcal{H}_1}\left(C\gamma_N^0 \right) = -\mathrm{i}\,\mathrm{Tr}_{\mathcal{H}_1}(CG_{\mathrm{h}}(0^-)).$$

This calculation is valid only for one-body operators. It is not possible to obtain the expectation value in the ground state of a generic two-body operator from the one-body Green's function. This is however the case for the ground state energy (the expectation value of the two-body Hamiltonian H_N in the ground state), as was first shown by Galiskii and Migdal [15]. Alternative formulae for the ground state energy are provided by the Luttinger-Ward formula [27] and the Klein's formula [24].

Theorem 36 (Galitskii-Migdal formula). *For all $N \geqslant 2$, the ground state energy can be recovered as*

$$E_N^0 = \frac{1}{2}\mathrm{Tr}_{\mathcal{H}_1}\left(-A_-^*\left(H_{N-1} - E_N^0 \right) A_- + \left(-\frac{1}{2}\Delta + v_{\mathrm{ext}} \right) A_-^* A_- \right) \tag{49}$$

$$= \frac{1}{2}\mathrm{Tr}_{\mathcal{H}_1}\left[\left(\frac{d}{d\tau} - \mathrm{i}\left(-\frac{1}{2}\Delta + v_{\mathrm{ext}} \right) \right) G_{\mathrm{h}}(\tau)\Big|_{\tau=0^-} \right]. \tag{50}$$

The proof of this theorem can be read in Section 6.10. Formula (50) is one way to obtain the right-hand side of (49), and is the one found in the original article [15]. There are however other ways to obtain (49) from the hole Green's function, without the use of derivative (which are cumbersome to evaluate numerically). One can for instance use the following equality, that we do not prove for the sake of brevity,

$$\mathrm{Tr}_{\mathcal{H}_1}\left(A_-^*\left(H_{N-1} + \mu - E_N^0 \right) A_- \right) = \lim_{\omega \to \infty} \omega^2 \mathrm{Tr}_{\mathcal{H}_1}\left(\mathrm{Re}\,\widetilde{G_{\mathrm{h}}}(\mu + \mathrm{i}\omega) \right).$$

3.2.3 The time-ordered Green's function G

It is often claimed in the physics literature that the main object of interest is neither the particle nor the hole Green's function, but the function

$$\mathcal{G}(\mathbf{r}t, \mathbf{r}'t') = \mathcal{G}_{\mathrm{p}}(\mathbf{r}t, \mathbf{r}'t') + \mathcal{G}_{\mathrm{h}}(\mathbf{r}t, \mathbf{r}'t'),$$

called the time-ordered Green's function, which can be seen as a convenient way to concatenate the information contained in the particle and hole Green's functions. Obviously, the time-ordered Green's function only depends on the time difference $\tau = t - t'$ and $\mathcal{G}(\mathbf{r}t, \mathbf{r}'t') = \mathcal{G}_{\mathrm{p}}(\mathbf{r}(t-t'), \mathbf{r}'0) + \mathcal{G}_{\mathrm{h}}(\mathbf{r}(t-t'), \mathbf{r}'0)$. In view of (38) and (45), our definition of the time-ordered Green's function therefore is the following.

Definition 37 (Green's function). *The (time-ordered) Green's function is the family of bounded operators $(G(\tau))_{\tau \in \mathbb{R}}$ defined as*

$$G(\tau) = G_{\mathrm{p}}(\tau) + G_{\mathrm{h}}(\tau) = -\mathrm{i}\Theta(\tau)\,A_+ \mathrm{e}^{-\mathrm{i}\tau(H_{N+1}-E_N^0)}A_+^* + \mathrm{i}\Theta(-\tau)\,A_-^* \mathrm{e}^{\mathrm{i}\tau(H_{N-1}-E_N^0)}A_-.$$

The following results straightforwardly follow from Propositions 28 and 34, as well as Lemmas 29 and 35. We recall that μ is a chemical potential of the electrons for the ground state Ψ_N^0 of the reference system, and that $E_N^0 - E_{N-1}^0 < \mu < E_{N+1}^0 - E_N^0$. In the following, we introduce some $C^\infty(\mathbb{R}_\omega)$ cut-off functions $\phi_\pm$ satisfying $0 \leqslant \phi_\pm \leqslant 1$, $\phi_+ + \phi_- = 1$, $\mathrm{Supp}(\phi_+) \subset (E_N^0 - E_{N-1}^0, +\infty)$ and $\mathrm{Supp}(\phi_-) \subset (-\infty, E_{N+1}^0 - E_N^0)$ (see Figure 3). These cut-off functions allow us to write properties of the Green's function in the time representation without specifying whether τ is positive or negative.
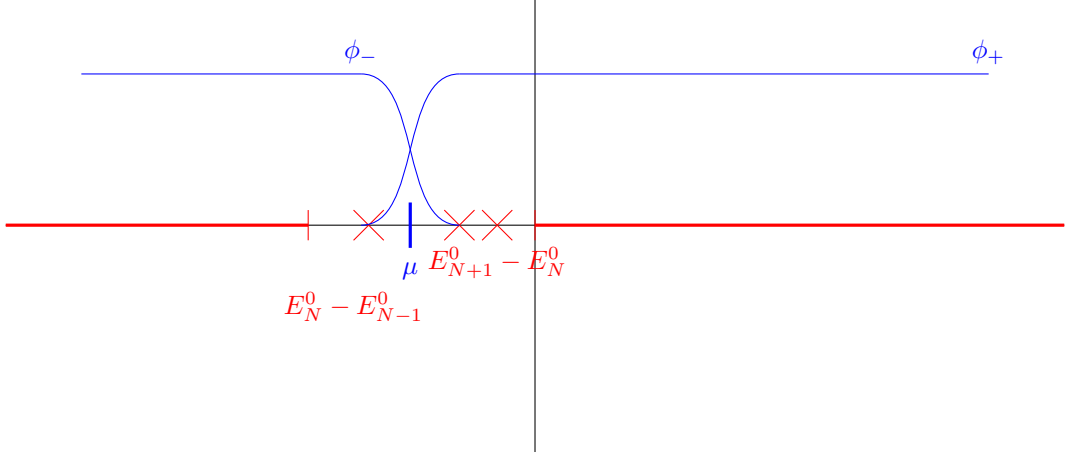
Figure 3: The cut-off functions $\phi_\pm$.

Proposition 38 (Properties of the Green's function). *The Fourier transform $\widehat{G} = \widehat{G_{\mathrm{p}}} + \widehat{G_{\mathrm{h}}}$ is in $H^{-s}(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$ for any $s > 1/2$. The operator-valued analytic function $\widetilde{G}$ defined on the physical Riemann sheet $\mathbb{C} \setminus (S_{\mathrm{p}} \cup S_{\mathrm{h}})$ by*

$$\forall z \in \mathbb{C} \setminus (S_{\mathrm{p}} \cup S_{\mathrm{h}}), \qquad \widetilde{G}(z) := A_+ \frac{1}{z - (H_{N+1} - E_N^0)} A_+^* + A_-^* \frac{1}{z - (E_N^0 - H_{N-1})} A_- \quad (51)$$

is such that

$$\lim_{\eta \to 0+} \phi_\pm \widetilde{G}(\cdot \pm \mathrm{i}\eta) = \phi_\pm \widehat{G} \quad \text{in } H^{-s}(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1)) \quad \text{for all } s > 1/2.$$

The function $\omega \mapsto \widetilde{G}(\mu + \mathrm{i}\omega)$ is real analytic from $\mathbb{R}_\omega$ to $\mathcal{B}(\mathcal{H}_1)$, and is in $L^p(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$ for all $p > 1$. Moreover, it satisfies the symmetry property

$$\forall \omega \in \mathbb{R}_\omega, \quad \operatorname{Re} \widetilde{G}(\mu + \mathrm{i}\omega) = \operatorname{Re} \widetilde{G}(\mu - \mathrm{i}\omega).$$

For any $f \in \mathcal{H}_1$, the function $\omega \mapsto \langle f | \operatorname{Re} \widetilde{G}(\mu + \mathrm{i}\omega) | f \rangle$ is in $L^1(\mathbb{R}_\omega)$, and

$$\int_{-\infty}^{+\infty} \left\langle f \left| \operatorname{Re} \widetilde{G}(\mu + \mathrm{i}\omega) \right| f \right\rangle \mathrm{d}\omega = -\pi \langle f | (\mathbb{1}_{\mathcal{H}_1} - 2\gamma_N^0) | f \rangle.$$

3.2.4 The spectral functions $\mathcal{A}_{\mathrm{p}}$, $\mathcal{A}_{\mathrm{h}}$ and $\mathcal{A}$

Spectral functions are essential tools to study many-body effects since they are concentrated on (subsets of) the particle and hole excitation sets.

Definition 39 (Spectral functions). *The* particle spectral function *is the operator-valued Borel measure on $\mathbb{R}_\omega$ defined by*

$$\forall b \in \mathscr{B}(\mathbb{R}_\omega), \qquad \mathcal{A}_{\mathrm{p}}(b) = -\frac{1}{\pi} \operatorname{Im} \widehat{G_{\mathrm{p}}}(b) = A_+ P_b^{H_{N+1} - E_N^0} A_+^*. \quad (52)$$

The hole spectral function *is similarly defined:*

$$\forall b \in \mathscr{B}(\mathbb{R}_\omega), \qquad \mathcal{A}_{\mathrm{h}}(b) = \frac{1}{\pi} \operatorname{Im} \widehat{G_{\mathrm{h}}}(b) = A_-^* P_b^{E_N^0 - H_{N-1}} A_-.$$

The time-ordered spectral function *is then obtained as $\mathcal{A} = \mathcal{A}_{\mathrm{p}} + \mathcal{A}_{\mathrm{h}}$.*

With those definitions, the following lemma is straightforward, and is usually referred to as the sum-rule for spectral functions (see for instance [11, Section 4.5]).

Proposition 40. *The spectral functions $\mathcal{A}_p$, $\mathcal{A}_h$ and $\mathcal{A}$ are $\mathcal{S}(\mathcal{H}_1)$-valued Borel measures on $\mathbb{R}_\omega$, with supports contained in S_p, S_h and $S_p \cup S_h$ respectively. For all $b \in \mathscr{B}(\mathbb{R}_\omega)$, $\mathcal{A}_p(b)$, $\mathcal{A}_h(b)$ and $\mathcal{A}(b)$ are bounded positive self-adjoint operators on $\mathcal{H}_1$ with norms lower or equal to 1. Moreover, $0 \leqslant \mathcal{A}_p(b_1) \leqslant \mathcal{A}_p(b_2)$ as self-adjoint operators when $b_1 \subset b_2$ (and similar inequalities for $\mathcal{A}_h$ and $\mathcal{A}$), and it holds*

$$\mathcal{A}_p(\mathbb{R}_\omega) = \mathbb{1}_{\mathcal{H}_1} - \gamma_N^0, \qquad \mathcal{A}_h(\mathbb{R}_\omega) = \gamma_N^0, \qquad \mathcal{A}(\mathbb{R}_\omega) = \mathbb{1}_{\mathcal{H}_1}.$$

Finally, the Plemelj formulae (14) allow us to recover the real part of the Green's functions from the spectral functions: $\operatorname{Re}\widehat{G_p} = \pi\mathfrak{H}(\mathcal{A}_p)$ and $\operatorname{Re}\widehat{G_h} = \pi\mathfrak{H}(\mathcal{A}_h)$. It therefore holds $\operatorname{Re}\widehat{G} = \pi\mathfrak{H}\mathcal{A}$.

3.3 Linear response operators

We study in this section the reducible polarizability operator χ, which can be defined from the so-called charge-fluctuation operator introduced in Section 3.3.1. We give a precise mathematical meaning to χ in Section 3.3.2, and prove Johnson's sum-rule [23] for χ in Section 3.3.3. We finally define the dynamically screened Coulomb interaction operator (see Section 3.3.4).

3.3.1 The charge-fluctuation operator ρ_H

The charge-fluctuation operator is defined, within the second quantization formalism, by (see [11, Equation (97)])

$$\rho_H(\mathbf{r}t) := \Psi_H^\dagger(\mathbf{r}t)\Psi_H(\mathbf{r}t) - \rho_N^0(\mathbf{r}),$$

so that the action of this operator on the N-body ground state is

$$
\begin{aligned}
\rho_H(\mathbf{r}t)|\Psi_N^0\rangle &= \left(\mathrm{e}^{\mathrm{i}t(H_N - E_N^0)}\right)\Psi^\dagger(\mathbf{r})\Psi(\mathbf{r})|\Psi_N^0\rangle - \rho_N^0(\mathbf{r})|\Psi_N^0\rangle \\
&= \left(\mathrm{e}^{\mathrm{i}t(H_N - E_N^0)}\right)\left(\Psi^\dagger(\mathbf{r})\Psi(\mathbf{r}) - \rho_N^0(\mathbf{r})\right)|\Psi_N^0\rangle.
\end{aligned}
\tag{53}
$$

In order to define more rigorously ρ_H, we need to introduce functional spaces of charge densities (the Coulomb space) and electrostatic potentials. The complex-valued Coulomb space

$$\mathcal{C} := \left\{ f \in \mathscr{S}'(\mathbb{R}^3, \mathbb{C}) \;\middle|\; \widehat{f} \in L^1_{\mathrm{loc}}(\mathbb{R}^3, \mathbb{C}), \; |\cdot|^{-1}\widehat{f}(\cdot) \in L^2(\mathbb{R}^3, \mathbb{C}) \right\}, \tag{54}$$

is endowed with the inner product

$$\langle f_1 | f_2 \rangle_{\mathcal{C}} = 4\pi \int_{\mathbb{R}^3} \frac{\overline{\widehat{f_1}(\mathbf{k})}\widehat{f_2}(\mathbf{k})}{|\mathbf{k}|^2} \, \mathrm{d}\mathbf{k},$$

where the normalization condition for the space-Fourier transform is chosen such that its restriction to $L^2(\mathbb{R}^3, \mathbb{C})$ is a unitary operator. The space $\mathcal{C}$ is a Hilbert space, and $L^{6/5}(\mathbb{R}^3, \mathbb{C}) \hookrightarrow \mathcal{C}$ thanks to the Hardy-Littlewood-Sobolev inequality (upon rewriting the products in Fourier space as convolutions). The dual of $\mathcal{C}$ (taking $L^2(\mathbb{R}^3, \mathbb{C})$ as a pivoting space) is

$$\mathcal{C}' := \left\{ v \in L^6(\mathbb{R}^3, \mathbb{C}) \;\middle|\; \nabla v \in \left(L^2(\mathbb{R}^3, \mathbb{C})\right)^3 \right\}, \tag{55}$$

endowed with the inner product

$$\langle V_1 | V_2 \rangle_{\mathcal{C}'} := \frac{1}{4\pi} \int_{\mathbb{R}^3} \overline{\nabla V_1} \cdot \nabla V_2 = \frac{1}{4\pi} \int_{\mathbb{R}^3} |\mathbf{k}|^2 \overline{\widehat{V_1}(\mathbf{k})}\, \widehat{V_2}(\mathbf{k}) \, \mathrm{d}\mathbf{k}.$$

We also introduce the Coulomb operator v_c, defined as the multiplication operator by $4\pi|\mathbf{k}|^{-2}$ in the Fourier representation, and its square root $v_c^{1/2}$, defined as the multiplication operator by $(4\pi)^{1/2}|\mathbf{k}|^{-1}$ in the Fourier representation. The following result, whose proof is a straightforward consequence of the above definitions, will be repeatedly used throughout this article.

Lemma 41. *The operator v_c defines a unitary operator from $\mathcal{C}$ to $\mathcal{C}'$. The operator $v_c^{1/2}$ defines a unitary operator from $\mathcal{C}$ to $\mathcal{H}_1$, as well as a unitary operator from $\mathcal{H}_1$ to $\mathcal{C}'$.*

It follows that the adjoint of the unitary operator $v_c : \mathcal{C} \to \mathcal{C}'$ is the unitary operator $v_c^* = v_c^{-1} : \mathcal{C}' \to \mathcal{C}$.

We are now able to reformulate the charge-fluctuation operator in the ground state as a well defined bounded operator. For $v \in C_c^\infty(\mathbb{R}^3, \mathbb{C})$, it formally holds

$$\left(\int_{\mathbb{R}^3} \left(\Psi^\dagger(\mathbf{r})\Psi(\mathbf{r}) - \rho_N^0(\mathbf{r}) \right) |\Psi_N^0\rangle\, v(\mathbf{r}) \mathrm{d}\mathbf{r} \right)(\mathbf{r}_1, \dots, \mathbf{r}_N) = \left[\left(\sum_{i=1}^N v(\mathbf{r}_i) \right) - \int_{\mathbb{R}^3} v \rho_N^0 \right] \Psi_N^0(\mathbf{r}_1, \dots \mathbf{r}_N).$$

In order to rewrite more rigorously this equality, we introduce the operator

$$\begin{aligned} B : \quad \mathcal{C}' &\to \mathcal{H}_N \\ v &\mapsto \left[\left(\sum_{i=1}^N v(\mathbf{r}_i) \right) - \langle v, \rho_N^0 \rangle_{\mathcal{C}',\mathcal{C}} \right] |\Psi_N^0\rangle, \end{aligned} \tag{56}$$

which is well defined since $\rho_N^0 \in L^{6/5}(\mathbb{R}^3, \mathbb{R})$ by Proposition 26. In fact, as made clear in Lemma 42 below, B is bounded. In view of (53), we can finally define the application to Ψ_N^0 of the charge-fluctuation operator $\rho_{\mathrm{H}}(t)$ as follows:

$$\rho_{\mathrm{H}}(t)|\Psi_N^0\rangle = \mathrm{e}^{\mathrm{i}t(H_N - E_N^0)} B. \tag{57}$$

Let us conclude this section by giving some properties of the operators introduced above (see Section 6.11 for the proof).

Lemma 42. *The operator B defined by (56) is a bounded operator from $\mathcal{C}'$ to $\mathcal{H}_N$. Its adjoint B^* is a bounded operator from $\mathcal{H}_N$ to $\mathcal{C}'$ which satisfies $B^*|\Psi_N^0\rangle = 0$. As a consequence, $\rho_{\mathrm{H}}|\Psi_N^0\rangle \in L^\infty(\mathbb{R}_t, \mathcal{B}(\mathcal{C}', \mathcal{H}_N))$, and $\left(\rho_{\mathrm{H}}|\Psi_N^0\rangle \right)^* \in L^\infty(\mathbb{R}_t, \mathcal{B}(\mathcal{H}_N, \mathcal{C}'))$.*

3.3.2 The (symmetrized) reducible polarizability operator χ

Definition of the reducible polarizability operator. The reducible polarizability operator $\chi(t, t')$ is the operator giving the response of the density of the system to perturbations of the external potential. It is formally defined by its kernel (see [11, Equation (96)])

$$\chi(\mathbf{r}t, \mathbf{r}'t') := -\mathrm{i} \left\langle \Psi_N^0 \middle| \mathcal{T} \{\rho_{\mathrm{H}}(\mathbf{r}t)\rho_{\mathrm{H}}(\mathbf{r}'t')\} \middle| \Psi_N^0 \right\rangle_{\mathcal{H}_N}. \tag{58}$$

In the above equation, ρ_{H} is the charge-fluctuation operator whose action on Ψ_N^0 is defined by (57), and $\mathcal{T}$ stands for the bosonic time-ordering operator:

$$\mathcal{T} \{A_1(t)A_2(t')\} = \left| \begin{array}{ll} A_1(t)A_2(t') & \text{if } t' < t, \\ A_2(t')A_1(t) & \text{if } t' > t. \end{array} \right.$$

In view of (57), the definition (58) of the kernel is formally equivalent to the following identity, stated for $t' < t$ (a similar equality being true for $t' > t$):

$$\begin{aligned} \int_{\mathbb{R}^3} \overline{f}\,(\chi(t, t')g) &= -\mathrm{i} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \overline{f}(\mathbf{r}) \left\langle \Psi_N^0 \middle| \rho_{\mathrm{H}}(\mathbf{r}t)\rho_{\mathrm{H}}(\mathbf{r}'t') \middle| \Psi_N^0 \right\rangle_{\mathcal{H}_N} g(\mathbf{r}')\, \mathrm{d}\mathbf{r}\, \mathrm{d}\mathbf{r}' \\ &= -\mathrm{i} \left\langle \int_{\mathbb{R}^3} f(\mathbf{r})\rho_{\mathrm{H}}(\mathbf{r}t)\Psi_N^0\, \mathrm{d}\mathbf{r} \middle| \int_{\mathbb{R}^3} g(\mathbf{r}')\rho_{\mathrm{H}}(\mathbf{r}'t')\Psi_N^0\, \mathrm{d}\mathbf{r}' \right\rangle_{\mathcal{H}_N} \\ &= -\mathrm{i} \left\langle \mathrm{e}^{\mathrm{i}t(H_N - E_N^0)} Bf \middle| \mathrm{e}^{\mathrm{i}t'(H_N - E_N^0)} Bg \right\rangle_{\mathcal{H}_N} \\ &= -\mathrm{i} \left\langle f \middle| B^* \mathrm{e}^{-\mathrm{i}(t - t')(H_N - E_N^0)} Bg \right\rangle_{\mathcal{C}'}. \end{aligned}$$

In order to interpret χ as giving the variation of the ground state density (an element of $\mathcal{C}$) generated by a variation of the external potential (an element of $\mathcal{C}'$), we rewrite the scalar product in $\mathcal{C}'$ as a duality braket between $\mathcal{C}'$ and $\mathcal{C}$:

$$\langle f_1 | f_2 \rangle_{\mathcal{C}'} = \langle \overline{f_1}, v_c^{-1} f_2 \rangle_{\mathcal{C}', \mathcal{C}}. \tag{59}$$

This motivates defining $\chi(t, t')$ as the bounded operator from $\mathcal{C}'$ to $\mathcal{C}$ given by

$$\chi(t, t') = -\mathrm{i} v_c^{-1} B^* \mathrm{e}^{-\mathrm{i}|t-t'|(H_N - E_N^0)} B.$$

In particular, $\chi(t, t')$ only depends on the time difference $t - t'$, and we write in the sequel $\chi(\tau) := \chi(\tau, 0)$:

$$\chi(\tau) = -\mathrm{i} v_c^{-1} B^* \mathrm{e}^{-\mathrm{i}|\tau|(H_N - E_N^0)} B. \tag{60}$$

It turns out to be useful to symmetrize the action of the polarizability operator using appropriate Coulomb operators. Recall that $B v_c^{1/2} \in \mathcal{B}(\mathcal{H}_1, \mathcal{H}_N)$ while $(B v_c^{1/2})^* = v_c^{-1/2} B^* \in \mathcal{B}(\mathcal{H}_N, \mathcal{H}_1)$.

Definition 43. *The symmetrized reducible polarizability operator* $\chi_{\mathrm{sym}} \in L^\infty(\mathbb{R}_\tau, \mathcal{B}(\mathcal{H}_1))$ *is defined by*

$$\forall \tau \in \mathbb{R}_\tau, \quad \chi_{\mathrm{sym}}(\tau) = v_c^{1/2} \chi(\tau) v_c^{1/2} = -\mathrm{i} v_c^{-1/2} B^* \mathrm{e}^{-\mathrm{i}|\tau|(H_N - E_N^0)} B v_c^{1/2}.$$

It is convenient to decompose the symmetrized reducible polarizability operator into two parts, namely its causal part and its anti-causal part:

$$\chi_{\mathrm{sym}}(\tau) = \chi_{\mathrm{sym}}^+(\tau) + \chi_{\mathrm{sym}}^-(\tau) \quad \text{with} \quad \chi_{\mathrm{sym}}^\pm(\tau) = \Theta(\pm\tau) \left(-\mathrm{i} v_c^{-1/2} B^* \mathrm{e}^{-\mathrm{i}|\tau|(H_N - E_N^0)} B v_c^{1/2} \right). \tag{61}$$

In the above expression, the Hamiltonian H_N can be replaced by

$$H_N^\sharp := H_N \big|_{\{\Psi_N^0\}^\perp}.$$

This is a consequence of Lemma 42 which shows that $\mathrm{Ran}(B) \subset \{\Psi_N^0\}^\perp$. Note that $H_N^\sharp - E_N^0 \geqslant E_N^1 - E_N^0$.

Properties of the symmetrized reducible polarizability operator. As rigorously stated below, the symmetrized polarizability operator has singularities at the energy differences corresponding to excitation energies for a system with a fixed number N of electrons, called neutral excitations in [11, Section 8]. We therefore introduce the neutral excitation set

$$S_0^+ := \sigma(H_N - E_N^0) \setminus \{0\} = \sigma\left(H_N^\sharp - E_N^0 \right),$$

its reflection $S_0^- := -S_0^+$ and $S_0 := S_0^+ \cup S_0^-$. Note that $S_0^+ \subset [E_N^1 - E_N^0, +\infty)$ so that $S_0^- \cap S_0^+ = \emptyset$.

As for Proposition 38, it turns out to be convenient to introduce appropriate cut-off functions. Consider $\phi_\pm^1$ such that ϕ_-^1 and ϕ_+^1 are in $C^\infty(\mathbb{R}_\omega)$ and satisfy $0 \leqslant \phi_\pm^1 \leqslant 1$, $\phi_+^1 + \phi_-^1 = 1$, $\mathrm{Supp}(\phi_+^1) \subset (-(E_N^1 - E_N^0), +\infty)$ and $\mathrm{Supp}(\phi_-^1) \subset (-\infty, E_N^1 - E_N^0)$ (see Figure 4).

Proposition 44. *The symmetrized reducible polarizability operator* χ_{sym} *satisfies the following properties:*

(1) $(\chi_{\mathrm{sym}}^+(\tau))_{\tau \in \mathbb{R}}$ *is a bounded causal operator on* $\mathcal{H}_1$ *while* $(\chi_{\mathrm{sym}}^-(\tau))_{\tau \in \mathbb{R}}$ *is a bounded anti-causal operator on* $\mathcal{H}_1$. *They satisfy the following symmetry properties:*

$$\forall \tau \in \mathbb{R}, \quad \chi_{\mathrm{sym}}(-\tau) = \chi_{\mathrm{sym}}(\tau) \quad \text{and} \quad \chi_{\mathrm{sym}}^+(\tau) = \chi_{\mathrm{sym}}^-(-\tau); \tag{62}$$
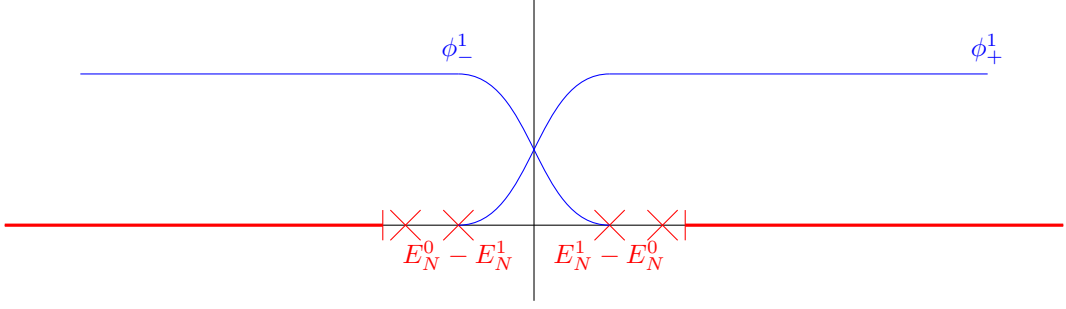
Figure 4: The cut-off functions $\phi_\pm^1$.

(2) the real and imaginary parts of the time-Fourier transforms of $\chi_{\text{sym}}^+, \chi_{\text{sym}}^-$ are respectively given by

$$\text{Re}\,\widehat{\chi_{\text{sym}}^\pm} = \pm v_c^{-1/2} B^* \text{p.v.} \left(\frac{1}{\cdot \mp (H_N^\sharp - E_N^0)} \right) B v_c^{1/2},$$

and

$$\text{Im}\,\widehat{\chi_{\text{sym}}^\pm} = -\pi v_c^{-1/2} B^* P^{\pm(H_N^\sharp - E_N^0)} B v_c^{1/2}.$$

In particular, $\text{Supp}\left(\text{Im}\,\widehat{\chi_{\text{sym}}^\pm}\right) \subset S_0^\pm$ and $\text{Supp}\left(\text{Im}\,\widehat{\chi_{\text{sym}}}\right) \subset S_0$;

(3) consider the $\mathcal{B}(\mathcal{H}_1)$-valued analytic functions $\widetilde{\chi_{\text{sym}}^+}, \widetilde{\chi_{\text{sym}}^-}$ and $\widetilde{\chi_{\text{sym}}}$ respectively defined by

$$\forall z \in \mathbb{C} \setminus S_0^\pm, \qquad \widetilde{\chi_{\text{sym}}^\pm}(z) := \pm v_c^{-1/2} B^* \frac{1}{z \mp (H_N^\sharp - E_N^0)} B v_c^{1/2},$$

and

$$\forall z \in \mathbb{C} \setminus S_0, \qquad \widetilde{\chi_{\text{sym}}}(z) := \widetilde{\chi_{\text{sym}}^+}(z) + \widetilde{\chi_{\text{sym}}^-}(z) = -v_c^{-1/2} B^* \frac{2(H_N^\sharp - E_N^0)}{(H_N^\sharp - E_N^0)^2 - z^2} B v_c^{1/2}. \quad (63)$$

It holds

$$\forall z \in \mathbb{C} \setminus S_0^+, \qquad \widetilde{\chi_{\text{sym}}^+}(z) = \widetilde{\chi_{\text{sym}}^-}(-z) = \left(\widetilde{\chi_{\text{sym}}^+}(\overline{z})\right)^*$$

and

$$\forall z \in \mathbb{C} \setminus S_0, \quad \widetilde{\chi_{\text{sym}}}(z) = \widetilde{\chi_{\text{sym}}}(-z) = \left(\widetilde{\chi_{\text{sym}}}(\overline{z})\right)^*.$$

The functions $\widetilde{\chi_{\text{sym}}^+}|_\mathbb{U}$ and $\widetilde{\chi_{\text{sym}}^-}|_\mathbb{L}$ are respectively the Laplace transforms of χ_{sym}^+ and χ_{sym}^-, and the following convergences hold in $H^{-s}(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$ for all $s > 1/2$:

$$\lim_{\eta \to 0^+} \widetilde{\chi_{\text{sym}}^\pm}(\cdot \pm \mathrm{i}\eta) = \widehat{\chi_{\text{sym}}^\pm}, \qquad \lim_{\eta \to 0^+} \phi_\pm^1 \widetilde{\chi_{\text{sym}}}(\cdot \pm \mathrm{i}\eta) = \phi_\pm^1 \widehat{\chi_{\text{sym}}};$$

(4) for all $\omega \in \left(-(E_N^1 - E_N^0), E_N^1 - E_N^0\right)$, $\widetilde{\chi_{\text{sym}}}(\omega) = \widehat{\chi_{\text{sym}}}(\omega)$ is a negative bounded self-adjoint operator on $\mathcal{H}_1$;

(5) for all $\omega \in \mathbb{R}$, $\widetilde{\chi_{\text{sym}}}(\mathrm{i}\omega)$ is a negative bounded self-adjoint operator on $\mathcal{H}_1$.

We omit the proof of Proposition 44 since the first three assertions are similar to those of Lemma 38, while the last two ones are direct consequences of (63).

On the integrability of $\widetilde{\chi_{\mathrm{sym}}}(\mathrm{i}\omega)$. As for the Green's function, $\omega \mapsto \widehat{\chi_{\mathrm{sym}}}(\omega)$ is difficult to study on the real-axis, and it is more convenient to study its analytical continuation $\widetilde{\chi_{\mathrm{sym}}}$ on the imaginary axis $\mathrm{i}\mathbb{R}$. This is possible thanks to the existence of the gap $(-(E_N^1 - E_N^0), E_N^1 - E_N^0)$ around 0. The representation provided in Proposition 44 allows one to directly deduce the integrability properties of the functions $\omega \mapsto \widetilde{\chi_{\mathrm{sym}}}(\mathrm{i}\omega)$ (as in Lemma 29).

Corollary 45. *The functions $\omega \mapsto \widetilde{\chi_{\mathrm{sym}}^{\pm}}(\mathrm{i}\omega)$ are real-analytic from $\mathbb{R}_\omega$ to $\mathcal{S}(\mathcal{H}_1)$, and are in $L^p(\mathbb{R}_\omega, \mathcal{S}(\mathcal{H}_1))$ for all $p > 1$. For any $f \in \mathcal{H}_1$, the function $\omega \mapsto \langle f | \widetilde{\chi_{\mathrm{sym}}}(\mathrm{i}\omega) | f \rangle$ is non-positive and in $L^1(\mathbb{R}_\omega)$, and it holds*

$$\int_{-\infty}^{+\infty} \langle f | \widetilde{\chi_{\mathrm{sym}}}(\mathrm{i}\omega) | f \rangle \mathrm{d}\omega = -2\pi \left\| B v_c^{1/2} f \right\|_{\mathcal{H}_N}^2. \tag{64}$$

3.3.3 The sum-rule for the reducible polarizability operator χ

The behavior of the reducible polarizability operator in the high imaginary-frequency regime is well understood. This asymptotic behavior is given by the so-called Johnson's sum-rule [23] or f-sum rule, the latter terminology being motivated in [11, Section 8.8] by the fact that it can formally be seen as some equality involving the first moment of $\mathrm{Im}\widehat{\chi_{\mathrm{sym}}}$. Knowing the large-$\omega$ behavior of $\widetilde{\chi_{\mathrm{sym}}}$ is important to design appropriate approximate operators, used in plasmon-pole models to avoid the numerical inversion of the dielectric operator (which is computationally expensive).

The fifth point of Proposition 44 implies that for all $\omega \in \mathbb{R}_\omega$, the operator $-\widetilde{\chi}(\mathrm{i}\omega) := -v_c^{-1/2} \widetilde{\chi_{\mathrm{sym}}}(\mathrm{i}\omega) v_c^{-1/2}$ defines a symmetric, continuous, non-negative sesquilinear form on $\mathcal{C}'$:

$$\forall (f, g) \in \mathcal{C}' \times \mathcal{C}', \qquad \langle \overline{f}, -\widetilde{\chi}(\mathrm{i}\omega) g \rangle_{\mathcal{C}', \mathcal{C}} = \left\langle Bf \left| \frac{2(H_N^\sharp - E_N^0)}{(H_N^\sharp - E_N^0)^2 + \omega^2} \right| Bg \right\rangle_{\mathcal{H}_N},$$

so that, formally,

$$\lim_{\omega \to \pm\infty} \langle \overline{f}, -\omega^2 \widetilde{\chi}(\mathrm{i}\omega) g \rangle_{\mathcal{C}', \mathcal{C}} = 2 \langle Bf | H_N^\sharp - E_N^0 | Bg \rangle_{\mathcal{H}_N} = 2 \left\langle \overline{f}, v_c^{-1} B^* \left(H_N^\sharp - E_N^0 \right) Bg \right\rangle_{\mathcal{C}', \mathcal{C}}.$$

The following theorem, whose proof is postponed until Section 6.12, confirms that this limit exists and allows one to identify it.

Theorem 46 (Johnson's sum rule). *The operator $2v_c^{-1} B^* (H_N^\sharp - E_N^0) B$ is bounded from $\mathcal{C}'$ to $\mathcal{C}$, and $2v_c^{-1} B^* (H_N^\sharp - E_N^0) B = -\mathrm{div} \left(\rho_N^0 \nabla \cdot \right)$. Moreover, the following weak convergence holds:*

$$\forall (f, g) \in \mathcal{C}' \times \mathcal{C}', \qquad \lim_{\omega \to \pm\infty} \left\langle \overline{f}, -\omega^2 \widetilde{\chi}(\mathrm{i}\omega) g \right\rangle_{\mathcal{C}', \mathcal{C}} = \left\langle \overline{f}, -\mathrm{div} \left(\rho_N^0 \nabla g \right) \right\rangle_{\mathcal{C}', \mathcal{C}} = \int_{\mathbb{R}^3} \rho_N^0 \overline{\nabla f} \cdot \nabla g.$$

For all $g \in \mathcal{C}'$ such that $\Delta g \in L^2(\mathbb{R}^3)$, the following strong convergence holds:

$$\lim_{\omega \to \pm\infty} \omega^2 \widetilde{\chi}(\mathrm{i}\omega) g = \mathrm{div} \left(\rho_N^0 \nabla g \right) \quad \text{in } \mathcal{C}.$$

3.3.4 The dynamically screened interaction operator W

As the name indicates, the two key operators in the GW method are on the one hand, the time-ordered Green's function G, and on the other hand, the so-called *dynamically screened interaction* operator W. The latter operator is defined as

$$W(\tau) = v_c \delta_0(\tau) + v_c^{1/2} \chi_{\mathrm{sym}}(\tau) v_c^{1/2}, \tag{65}$$

where v_c is the Coulomb operator introduced in Lemma 41. It is convenient to split W into a local-in-time exchange contribution $v_c \delta_0(\tau)$ (although this is not obvious at this stage, (98) below

shows that $v_c \delta_0(\tau)$ can be interpreted as an exchange term), and a nonlocal-in-time correlation contribution:

$$W(\tau) = v_c \delta_0(\tau) + W_c(\tau) \quad \text{with} \quad W_c(\tau) := v_c \chi(\tau) v_c = v_c^{1/2} \chi_{\text{sym}}(\tau) v_c^{1/2}. \tag{66}$$

The properties of the operator $W_c(\tau) \in \mathcal{B}(\mathcal{C}, \mathcal{C}')$ therefore readily follow from the properties of the operators $v_c^{1/2}$ and $\chi_{\text{sym}}(\tau)$ established in Lemma 41 and Proposition 44.

3.4 The self-energy operator Σ

We give in this section the definition of the self-energy operator Σ using the Dyson equation (see (72) below). Let us emphasize that, while the Dyson equation provides a definition of Σ in terms of Green's functions, numerical methods work the other way round: an approximation of the Green's function G is obtained from the Dyson equation (72), using an approximation of the self-energy operator Σ. This approach is made precise in Section 4.

3.4.1 The non-interacting Hamiltonian H_0 and associated Green's function G_0

The self-energy operator is defined as the difference between the inverse of the exact Green's function G and the inverse of some reference Green's function G_0. The reference Green's function is the resolvent of a mean-field non-interacting Hamiltonian. There are several possible choices for this operator, discussed in Remark 49 below. In order to remain as general as possible, we introduce a one-body operator h_1 acting on $\mathcal{H}_1$, with domain $H^2(\mathbb{R}^3)$, real-valued (in the sense that $h\psi$ is real-valued whenever ψ is real-valued), and such that $\sigma_{\text{ess}}(h_1) = [0, \infty)$. The corresponding effective non-interacting N-body Hamiltonian is defined on $\mathcal{H}_N$ by

$$H_{0,N} = \sum_{i=1}^{N} h_1(\mathbf{r}_i).$$

We define

$$\varepsilon_k := \inf_{V_k \subset \mathcal{V}_k} \sup_{v \in V_k \setminus \{0\}} \frac{\langle v|h_1|v \rangle}{\langle v|v \rangle},$$

where $\mathcal{V}_k$ is the set of the subspaces of $H^1(\mathbb{R}^3)$ of dimension k. Recall that $\varepsilon_k \leqslant 0$ and that if $\varepsilon_k < 0$, then h_1 has at least k negative eigenvalues (counting multiplicities) and ε_k is the kth smallest eigenvalue of h_1 (still counting multiplicities). We make the following assumption in the sequel.

Hyp. 3: The one-body Hamiltonian h_1 has at least N negative eigenvalues, and $\varepsilon_N < \varepsilon_{N+1}$.

This assumption implies that there is a gap between the Nth eigenvalue and the $(N+1)^{\text{st}}$ eigenvalue (or the bottom of the essential spectrum if h_1 has only N non-positive eigenvalues).

Let us denote by $(\phi_1, \cdots, \phi_N)$ an orthonormal family of eigenvectors of h_1 associated with the eigenvalues $\varepsilon_1, \cdots, \varepsilon_N$. Without loss of generality, we can assume that the ϕ_k's are real-valued. The ground state energy of $H_{0,N}$ is $E_{0,N}^0 = \varepsilon_1 + \ldots + \varepsilon_N$. The condition $\varepsilon_N < \varepsilon_{N+1}$ ensures that $E_{0,N}^0$ is a non-degenerate eigenvalue of $H_{0,N}$ and that the normalized ground state $\Phi_N^0 = \phi_1 \wedge \cdots \wedge \phi_N$ of $H_{0,N}$ is unique up to a global phase. We introduce the one-body mean-field density matrix

$$\gamma_{0,N}^0(\mathbf{r}, \mathbf{r}') := \sum_{k=1}^{N} \phi_k(\mathbf{r}) \phi_k(\mathbf{r}'). \tag{67}$$

This function can be seen as the kernel of the spectral projector $\mathbb{1}_{(-\infty, \mu_0)}(h_1)$, where μ_0 is any real number in the range $(\varepsilon_N, \varepsilon_{N+1})$ (it is an admissible Fermi level for the ground state of the non-interacting effective Hamiltonian $H_{0,N}$). The density of the non-interacting system is denoted

by $\rho_{0,N}^0$. Results similar to the ones stated in Proposition 26 for $\rho_{0,N}^0$, $\gamma_{0,N}^0$, ... hold true. Finally, similarly as in Section 3.2, we introduce

$$A_{0,+}^*(f) = a^\dagger(f)|\Phi_N^0\rangle \quad \text{and} \quad A_{0,-}(f) = a(\overline{f})|\Phi_N^0\rangle.$$

Definition 47 (Reference non-interacting Green's functions)**.** *The reference particle, hole and time-ordered non-interacting Green's functions are respectively defined as*

$$G_{0,\mathrm{p}}(\tau) = -\mathrm{i}\Theta(\tau)A_{0,+}\mathrm{e}^{-\mathrm{i}\tau(H_{0,N+1}-E_{0,N}^0)}A_{0,+}^*, \qquad G_{0,\mathrm{h}}(\tau) = \mathrm{i}\Theta(-\tau)A_{0,-}^*\,\mathrm{e}^{\mathrm{i}\tau(H_{0,N-1}-E_{0,N}^0)}A_{0,-},$$

and $G_0(\tau) = G_{0,\mathrm{p}}(\tau) + G_{0,\mathrm{h}}(\tau)$.

Results similar to Propositions 28, 34 and 38 hold for these operators, but we do not write them explicitly for the sake of brevity. However, it should be noted that, in the non-interacting case, the Green's functions have simple explicit expressions in terms of h_1 (see Section 6.13 for the proof).

Proposition 48. *It holds*

$$G_{0,\mathrm{p}}(\tau) = -\mathrm{i}\Theta(\tau)\left(\mathbb{1}_{\mathcal{H}_1} - \gamma_{0,N}^0\right)\mathrm{e}^{-\mathrm{i}\tau h_1} \quad \text{and} \quad G_{0,\mathrm{h}}(\tau) = \mathrm{i}\Theta(-\tau)\gamma_{0,N}^0\mathrm{e}^{-\mathrm{i}\tau h_1}.$$

In particular, for any $z \in \mathbb{C} \setminus \sigma(h_1)$,

$$\widetilde{G_{0,\mathrm{p}}}(z) = \left(\mathbb{1}_{\mathcal{H}_1} - \gamma_{0,N}^0\right)(z - h_1)^{-1} \quad \text{and} \quad \widetilde{G_{0,\mathrm{h}}}(z) = \gamma_{0,N}^0(z - h_1)^{-1}. \tag{68}$$

Hence,

$$\widetilde{G_0}(z) = (z - h_1)^{-1} \tag{69}$$

is the resolvent of the one-body operator h_1.

Remark 49 (On the choice of G_0)**.** *There are several possible choices for the one-body operator h_1, although this choice is not really properly discussed in the literature to our knowledge. The first option, which is used in the original derivation of the GW method [18], consists in choosing*

$$h_1 = -\frac{1}{2}\Delta + v_{\mathrm{ext}} + \rho_N^0 * |\cdot|^{-1}, \tag{70}$$

where ρ_N^0 is the exact ground state density. Another option (see for instance [11, page 112]) is to consider a one-body operator whose associated ground state density is (as close as possible to) the exact ground state density ρ_N^0. The motivation is that, in this case, the self-energy should be smaller. The Kohn-Sham [25] model formally satisfies this requirement. The associated one-body operator reads

$$h_1 = -\frac{1}{2}\Delta + v_{\mathrm{ext}} + \rho_N^0 * |\cdot|^{-1} + v_{\mathrm{xc}}\left[\rho_N^0\right], \tag{71}$$

where v_{xc} is the (exact) exchange-correlation potential. In practice, approximations of ρ_N^0 and $v_{\mathrm{xc}}\left[\rho_N^0\right]$ are computed by means of a Kohn-Sham LDA or GGA calculation [25, 32]. This is believed to provide a sufficiently accurate approximation of the exact ground state density which does not spoil the results subsequently obtained by GW calculations.

3.4.2 The dynamical Hamiltonian $\widetilde{H}(z)$

In view of (69), it is natural to introduce the inverse of the time-ordered Green's function, which will correspond to some dynamical one-body Hamiltonian. More precisely, we would like to define, at least for each $z \in \mathbb{C} \setminus \mathbb{R}$, a one-body operator $\widetilde{H}(z)$ such that

$$\widetilde{G}(z) := \left(z - \widetilde{H}(z)\right)^{-1}, \quad \text{or equivalently,} \quad \widetilde{H}(z) = z - \left(\widetilde{G}(z)\right)^{-1}.$$

The following proposition, proved in Section 6.14, shows that such a definition makes sense.

Proposition 50. *Let $z \in \mathbb{C} \setminus \mathbb{R}$. The operator $\widetilde{G}(z)$ is an invertible operator from $\mathcal{H}_1$ onto some vector subspace $\widetilde{D}(z)$ of $\mathcal{H}_1$. Moreover, $\widetilde{D}(z)$ is dense in $\mathcal{H}_1$, $\widetilde{D}(z) \subset H^2(\mathbb{R}^3)$, and $\widetilde{H}(z)$ is a well-defined closed operator with domain $\widetilde{D}(z)$.*

Remark 51. *We do not know whether the equality $\widetilde{D}(z) = H^2(\mathbb{R}^3)$ is true, nor do we know whether $\widetilde{D}(z_1) = \widetilde{D}(z_2)$ for $z_1 \neq z_2$.*

3.4.3 Definition of the self-energy operator Σ from the Dyson equation

We are now able to define the exact self-energy operator $\widetilde{\Sigma}$ via the Dyson equation. Note that we do not define the self-energy in the time domain, but consider only $\widetilde{\Sigma}(z)$ (as in [11, Section 5.1]).

Definition 52 (Self-energy)**.** *The self-energy operator is defined as*

$$\forall z \in \mathbb{C} \setminus \mathbb{R}, \qquad \widetilde{\Sigma}(z) := \widetilde{G_0}(z)^{-1} - \widetilde{G}(z)^{-1} = (z - h_1) - \left(z - \widetilde{H}(z) \right) = \widetilde{H}(z) - h_1, \qquad (72)$$

where h_1 is the one-body mean-field Hamiltonian introduced in Section 3.4.1.

The operator $\widetilde{\Sigma}(z)$ is the difference between the one-body dynamical Hamiltonian and the reference one-body mean-field Hamiltonian h_1. With this writing, $\widetilde{\Sigma}(z)$ can be seen as the correction term to be added to the reference one-body Hamiltonian in order to obtain the dynamical mean-field one-body Hamiltonian:

$$\widetilde{H}(z) = h_1 + \widetilde{\Sigma}(z).$$

4 The GW approximation for finite systems

4.1 $\mathbf{G_0W^0}$, self-consistent $\mathrm{GW^0}$, self-consistent GW, and all that

4.1.1 The GW equations

We now turn to the GW approximation for finite systems. The purpose of the GW approximation is to estimate the time-ordered Green's function G via the Dyson formula (72). Instead of using (72) to define the self-energy $\widetilde{\Sigma}(z)$, we use this equation *with some approximation $\widetilde{\Sigma}^{\mathrm{GW}}(z)$ of $\widetilde{\Sigma}(z)$* to obtain an approximation $\widetilde{G}^{\mathrm{GW}}(z)$ of the time-ordered Green's function via

$$\left(\widetilde{G}^{\mathrm{GW}} \right)^{-1} (z) = z - \left(h_1 + \widetilde{\Sigma}^{\mathrm{GW}}(z) \right). \qquad (73)$$

Using the Dyson equation to *define* the time-ordered Green's function is only possible if an alternative expression of the self-energy operator is available. Such an expression was formally obtained by Hedin in 1965 (see [18]). The GW approximation consists in replacing the so-called vertex function in Hedin's equations by a tensor product of Dirac masses.

The original GW equations were derived on the time domain and on the frequency domain. However, as noticed several times in Section 3, the operators involved in the GW equations are not smooth on these axes. It turns out that it is formally possible to recast the equations on some imaginary axis using Theorem 24. This approach, first introduced by Rojas, Godby and Needs [36] (see also [34]), is now known under the name of the "analytic continuation method". For reasons that we will explain throughout this section, these equations are recast as follows within our mathematical framework.

Definition 53 (GW equations on the imaginary axis of the frequency domain)**.**
Find $\widetilde{G^{\mathrm{GW}}}(\mu + \mathrm{i}\cdot) \in L^2(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}))$ *solution of the system*

$$\widetilde{P_{\mathrm{sym}}^{\mathrm{GW}}}(\mathrm{i}\omega) = \frac{1}{2\pi} v_c^{1/2} \left(\int_{-\infty}^{\infty} \widetilde{G^{\mathrm{GW}}}\big(\mu + \mathrm{i}(\omega + \omega')\big) \odot \widetilde{G^{\mathrm{GW}}}(\mu + \mathrm{i}\omega') \, \mathrm{d}\omega' \right) v_c^{1/2}, \tag{74a}$$

$$\widetilde{\chi_{\mathrm{sym}}^{\mathrm{GW}}}(\mathrm{i}\omega) = \left(\mathbb{1}_{\mathcal{H}} - \widetilde{P_{\mathrm{sym}}^{\mathrm{GW}}}(\mathrm{i}\omega) \right)^{-1} - \mathbb{1}_{\mathcal{H}_1}, \tag{74b}$$

$$\widetilde{W_c^{\mathrm{GW}}}(\mathrm{i}\omega) = v_c^{1/2} \widetilde{\chi_{\mathrm{sym}}^{\mathrm{GW}}}(\mathrm{i}\omega) v_c^{1/2}, \tag{74c}$$

$$\widetilde{\Sigma^{\mathrm{GW}}}(\mu + \mathrm{i}\omega) = K_x - \frac{1}{2\pi} \int_{-\infty}^{\infty} \widetilde{G^{\mathrm{GW}}}\big(\mu + \mathrm{i}(\omega - \omega')\big) \odot \widetilde{W_c^{\mathrm{GW}}}(\mathrm{i}\omega') \, \mathrm{d}\omega', \tag{74d}$$

$$\widetilde{G^{\mathrm{GW}}}(\mu + \mathrm{i}\omega) = \left[\mu + \mathrm{i}\omega - \left(h_1 + \widetilde{\Sigma^{\mathrm{GW}}}(\mu + \mathrm{i}\omega) \right) \right]^{-1}, \tag{74e}$$

where h_1 is the one-body operator defined in (70) and where K_x is the integral operator on $\mathcal{H}_1$ with kernel

$$K_x(\mathbf{r}, \mathbf{r}') := -\frac{\gamma_{0,N}^0(\mathbf{r}, \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|},$$

where $\gamma_{0,N}^0$ was defined in (67).

Remark 54. *In the* GW *equations (74), the chemical potential μ is supposed to be known a priori.*

The GW equations (74) would be the natural equations to work with from a mathematical viewpoint (they are formally equivalent to the original Hedin's GW equations). However, we were not able to study (74) for reasons detailed in Remark 55 below.

As one can directly see, the equations involve quite a large number of operators, which all have a physical significance. The operator $\widetilde{P_{\mathrm{sym}}^{\mathrm{GW}}}$ is the GW approximation of the symmetric irreducible polarizability operator, the operator $\widetilde{\chi_{\mathrm{sym}}^{\mathrm{GW}}}$ is the GW approximation of the symmetric reducible polarizability operator, the operator $\widetilde{W^{\mathrm{GW}}}$ is the GW approximation of the dynamically screened Coulomb interaction operator, and finally $\widetilde{\Sigma^{\mathrm{GW}}}$ is the GW approximation of the self-energy operator. We recognize in Equation (74e) the Dyson equation. The name "GW" comes from Equation (74d).

4.1.2 Different levels of GW approximation

As mentioned below (see Remark 55), we were not able to study the full self-consistent problem (74). We will therefore restrict ourselves to the so-called G_0W^0 and GW^0 approximations. We explain in this section how these different models are obtained.

(i) In the fully self-consistent GW (sc-GW) approximation, we assume that the full problem (74) is well-posed, so that there exists a (unique) solution $\widetilde{G^{\mathrm{GW}}}$. It is then solved self-consistently: the idea is to start from some trial Green's function, and keep updating it with (74) until convergence. This method is for instance used in [7, 8, 26, 37, 41]. It was implemented only quite recently due to its high numerical cost (one needs to perform the inversion in (74b) at each iteration).

(ii) In the so-called self-consistent GW^0 approximation, or simply GW^0 approximation, only the Green's function (and not the screened Coulomb operator) is updated in (74d) (see for instance [42, 46]). This partial update not only speeds up the calculation (the inversion in (74b) is only performed once), but is sometimes in better agreement with experimental results than the sc-GW approximation. This is the model that we study in Section 4.3.

(iii) Finally, most works simply consider the G_0W^0 approximation, where only one iteration of the sc-GW (or equivalently one iteration of GW^0) is performed. This model is very popular

due to its relatively low computational cost, and provides already very satisfactory results (see for instance [4]).

Let us also emphasize that it is unclear that a solution of the fully self-consistent GW model is a better approximation in any sense to the exact Green's function than a non self-consistent approximation such as the one obtained by the G_0W^0 approximation. This is discussed in [11, Section 9.8], where the author also comments on the possibilities to update the effective one-body operator $h_1 + K_x$ along the iterations.

Remark 55. *We do not know how to give a proper mathematical meaning to Equation (74a). More specifically, one would like to define, for a reasonable choice of Green's function $\widetilde{G^{\mathrm{app}}}$, the operator*

$$\forall \omega \in \mathbb{R}_\omega, \quad \widetilde{P_{\mathrm{sym}}}[G^{\mathrm{app}}](\mathrm{i}\omega) := \frac{1}{2\pi} v_c^{1/2} \left(\int_{-\infty}^\infty \widetilde{G^{\mathrm{app}}}\big(\mu + \mathrm{i}(\omega + \omega')\big) \odot \widetilde{G^{\mathrm{app}}}(\mu + \mathrm{i}\omega') \, \mathrm{d}\omega' \right) v_c^{1/2},$$

and we would like this operator to be a self-adjoint bounded negative operator on $\mathcal{H}_1$. It is the case for instance when $\widetilde{G^{\mathrm{app}}}$ is the non-interacting Hamiltonian $\widetilde{G_0}$ defined in (69) (see Proposition 59 and Remark 64), or when $\widetilde{G^{\mathrm{app}}}$ is the exact Green's function defined in (51) (this fact can be proved by adapting the arguments given in Section 4.2.2). We were not able to obtain this result for a generic class of approximate Green's functions $\widetilde{G^{\mathrm{app}}}$, say $\widetilde{G^{\mathrm{app}}}$ of the form (74e) with $\widetilde{\Sigma^{\mathrm{GW}}}(\mu + \mathrm{i}\omega)$ in a small ball of $L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$.

For this reason, we will not study the self-consistent GW equation (74).

4.2 The operator $\widetilde{W^0}$ and the random phase approximation

The remainder of this section is devoted to the study of the GW^0 approximation (which includes the G_0W^0 approximation), which amounts to study the two equations (74d)-(74e) with a specific fixed choice of the screening operator W^0. This approximation bypasses the difficulties mentioned in Remark 55. In order to present and study the GW^0 approximation, one must first define the operator W^0.

4.2.1 The RPA irreducible polarizability operator $\widetilde{P^0}$

The GW approximation of the *irreducible polarizability operator P* is formally defined as

$$P^{\mathrm{GW}}(\mathbf{r}, \mathbf{r}', \tau) = -\mathrm{i}G(\mathbf{r}, \mathbf{r}', \tau)G(\mathbf{r}', \mathbf{r}, -\tau). \tag{75}$$

When the Green's function G is the non-interacting one G_0 defined in (47), this also corresponds to the so-called random phase approximation of the reducible polarizability operator (compare for instance (83) with the expression in [6]). We therefore define

$$P^0(\mathbf{r}, \mathbf{r}', \tau) := -\mathrm{i}G_0(\mathbf{r}, \mathbf{r}', \tau)G_0(\mathbf{r}', \mathbf{r}, -\tau).$$

This operator is expected to have properties similar to the operator χ defined in Section 3.3.2. In particular, $P^0(\tau)$ is expected to be a bounded operator from $\mathcal{C}'$ to $\mathcal{C}$. It is therefore more convenient to work with its symmetrized counterpart $P_{\mathrm{sym}}^0(\tau) := v_c^{1/2} P^0(\tau) v_c^{1/2}$, which is expected to be a bounded operator on $\mathcal{H}_1$. It is possible to decompose P_{sym}^0 as $P_{\mathrm{sym}}^0 = P_{\mathrm{sym}}^{0,+} + P_{\mathrm{sym}}^{0,-}$ where, using the kernel-product $\odot$ defined in Section 2.4, and the explicit expressions of $G_{0,\mathrm{p}}$ and $G_{0,\mathrm{h}}$ given in Proposition 48,

$$P_{\mathrm{sym}}^{0,+}(\tau) = -\mathrm{i}\Theta(\tau) v_c^{1/2} G_{0,\mathrm{p}}(\tau) \odot G_{0,\mathrm{h}}(-\tau) v_c^{1/2} \tag{76}$$

$$= -\mathrm{i}\Theta(\tau) v_c^{1/2} \left(\left(\mathbb{1}_{\mathcal{H}_1} - \gamma_{0,N}^0\right) \mathrm{e}^{-\mathrm{i}\tau h_1} \odot \gamma_{0,N}^0 \mathrm{e}^{\mathrm{i}\tau h_1} \right) v_c^{1/2} \tag{77}$$

and

$$P_{\mathrm{sym}}^{0,-}(\tau) = -\mathrm{i}\Theta(-\tau)v_c^{1/2}G_{0,\mathrm{h}}(\tau) \odot G_{0,\mathrm{p}}(-\tau)v_c^{1/2}$$
$$= -\mathrm{i}\Theta(-\tau)v_c^{1/2}\left(\gamma_{0,N}^0 \mathrm{e}^{-\mathrm{i}\tau h_1} \odot \left(\mathbb{1}_{\mathcal{H}_1} - \gamma_{0,N}^0\right)\mathrm{e}^{\mathrm{i}\tau h_1}\right)v_c^{1/2}.$$

Actually, with this definition, we were not able to give a meaning to $P_{\mathrm{sym}}^{0,-}$ (it may not be a bounded operator on $\mathcal{H}_1$). We therefore prefer to use the modified kernel-product $\widetilde{\odot}$ defined in Remark 19. Our correct mathematical definition for $P_{\mathrm{sym}}^{0,-}$ then is

$$P_{\mathrm{sym}}^{0,-}(\tau) = -\mathrm{i}\Theta(-\tau)v_c^{1/2}G_{0,\mathrm{h}}(\tau) \,\widetilde{\odot}\, G_{0,\mathrm{p}}(-\tau)v_c^{1/2} \tag{78}$$
$$= -\mathrm{i}\Theta(-\tau)v_c^{1/2}\left(\gamma_{0,N}^0 \mathrm{e}^{-\mathrm{i}\tau h_1} \,\widetilde{\odot}\, \left(\mathbb{1}_{\mathcal{H}_1} - \gamma_{0,N}^0\right)\mathrm{e}^{\mathrm{i}\tau h_1}\right)v_c^{1/2}. \tag{79}$$

As will be shown in Lemma 56, this amounts to defining $P^{0,-}(\tau) = P^{0,+}(-\tau)$. We recall that $\gamma_{0,N}^0$ is the orthogonal projector on the vector space spanned by the eigenvectors of h_1 associated with the lowest N eigenvalues (see (67)), so that

$$\gamma_{0,N}^0 = \sum_{k=1}^{N} |\phi_k\rangle\langle\phi_k|, \tag{80}$$

where $h_1\phi_k = \varepsilon_k\phi_k$, and the eigenfunctions ϕ_k are real-valued and orthonormal. The following result shows that our definitions make sense, and gives explicit formulae for $P^{0,+}$ (see Section 6.15 for the proof).

Lemma 56. *The family $\left(P_{\mathrm{sym}}^{0,+}(\tau)\right)_{\tau\in\mathbb{R}_\tau}$ defined by (76) is a bounded causal operator on $\mathcal{H}_1$, while $\left(P_{\mathrm{sym}}^{0,-}(\tau)\right)_{\tau\in\mathbb{R}_\tau}$ defined by (78) is a bounded anti-causal operator on $\mathcal{H}_1$. It holds $P_{\mathrm{sym}}^{0,-}(\tau) = P_{\mathrm{sym}}^{0,+}(-\tau)$ and*

$$P_{\mathrm{sym}}^{0,+}(\tau) = -\mathrm{i}\Theta(\tau)\sum_{k=1}^{N} v_c^{1/2}\phi_k\left(\mathbb{1}_{\mathcal{H}_1} - \gamma_{0,N}^0\right)\mathrm{e}^{-\mathrm{i}\tau(h_1-\varepsilon_k)}\left(\mathbb{1}_{\mathcal{H}_1} - \gamma_{0,N}^0\right)\phi_k v_c^{1/2}. \tag{81}$$

Remark 57. *For $1 \leqslant k \leqslant N$, the notation ϕ_k in (81) refers to the multiplication operator by the function ϕ_k. It is a bounded operator from $\mathcal{C}'$ to $\mathcal{H}_1$, and from $\mathcal{H}_1$ to $\mathcal{C}$ (see the proof of Lemma 56). The operator $\phi_k v_c^{1/2}$ is bounded on $\mathcal{H}_1$, and one can check that its adjoint on $\mathcal{H}_1$ is $(\phi_k v_c^{1/2})^* := v_c^{1/2}\phi_k$.*

The properties of the Laplace and Fourier transforms of $P_{\mathrm{sym}}^{0,+}$ are easily deduced from (81) using Proposition 13 and Lemma 14.

Proposition 58. *The function $z \mapsto \widetilde{P_{\mathrm{sym}}^{0,+}}(z)$ is analytic on the upper half-plane $\mathbb{U}$, and can be analytically continued to the lower half-plane $\mathbb{L}$ through the semi-real line $(-\infty, \varepsilon_{N+1} - \varepsilon_N)$. For all $z \in \mathbb{C} \setminus [\varepsilon_{N+1} - \varepsilon_N, \infty)$,*

$$\widetilde{P_{\mathrm{sym}}^{0,+}}(z) = \sum_{k=1}^{N} v_c^{1/2}\phi_k\left(\frac{\mathbb{1}_{\mathcal{H}_1} - \gamma_{0,N}^0}{z - h_1 + \varepsilon_k}\right)\phi_k v_c^{1/2}. \tag{82}$$

Moreover $\widetilde{P_{\mathrm{sym}}^{0,+}}(\cdot + \mathrm{i}\eta)$ converges to $\widehat{P_{\mathrm{sym}}^{0,+}}$ in $H^{-1}(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$ as $\eta \to 0^+$, with

$$\mathrm{Re}\,\widehat{P_{\mathrm{sym}}^{0,+}} = \mathrm{p.v.}\left(\sum_{k=1}^{N} v_c^{1/2}\phi_k\left(\frac{\mathbb{1}_{\mathcal{H}_1} - \gamma_{0,N}^0}{\cdot - h_1 + \varepsilon_k}\right)\phi_k v_c^{1/2}\right)$$

and

$$\mathrm{Im}\,\widehat{P_{\mathrm{sym}}^{0,+}} = -\pi\left(\sum_{k=1}^{N} v_c^{1/2}\phi_k\left(\mathbb{1}_{\mathcal{H}_1} - \gamma_{0,N}^0\right)P^{h_1-\varepsilon_k}\phi_k v_c^{1/2}\right).$$

It also holds

$$\forall z \in \mathbb{C} \setminus [\varepsilon_{N+1} - \varepsilon_N, \infty), \quad \widetilde{P_{\mathrm{sym}}^{0,-}}(z) = \widetilde{P_{\mathrm{sym}}^{0,+}}(-z),$$

so that, for $z \in \mathbb{U} \cup \mathbb{L} \cup (-(\varepsilon_{N+1} - \varepsilon_N), \varepsilon_{N+1} - \varepsilon_N)$,

$$\widetilde{P_{\mathrm{sym}}^0}(z) = -2 \sum_{k=1}^{N} v_c^{1/2} \phi_k (\mathbb{1}_{\mathcal{H}_1} - \gamma_{0,N}^0) \left(\frac{h_1 - \varepsilon_k}{(h_1 - \varepsilon_k)^2 - z^2} \right) (\mathbb{1}_{\mathcal{H}_1} - \gamma_{0,N}^0) \phi_k v_c^{1/2}. \qquad (83)$$

The properties of $\widetilde{P_{\mathrm{sym}}^{0,+}}$ and of $\widetilde{P_{\mathrm{sym}}^{0,-}}$ can be directly read off from the previous expressions. For instance, we see that $\mathrm{Im}\, \widetilde{P_{\mathrm{sym}}^{0,+}}$ and $\mathrm{Im}\, \widetilde{P_{\mathrm{sym}}^{0,-}}$ are negative operator-valued measures, with support in $(\varepsilon_{N+1} - \varepsilon_N, \infty)$ and $(-\infty, -(\varepsilon_{N+1} - \varepsilon_N))$ respectively. For ω in the real gap $(-(\varepsilon_{N+1} - \varepsilon_N), \varepsilon_{N+1} - \varepsilon_N)$, we see that $\widetilde{P_{\mathrm{sym}}^{0,\pm}}(\omega) = \mathrm{Re}\, \widetilde{P_{\mathrm{sym}}^{0,\pm}}(\omega)$ is a negative bounded self-adjoint on $\mathcal{H}_1$.

For our purpose, we only need to know the behavior of $\widetilde{P_{\mathrm{sym}}^0}$ on the imaginary axis $\mathrm{i}\mathbb{R}_\omega$. We summarize the corresponding most important results in the following proposition (see Section 6.16 for the proof).

Proposition 59. *It holds*

$$\forall \omega \in \mathbb{R}_\omega, \quad \widetilde{P_{\mathrm{sym}}^0}(\mathrm{i}\omega) = -2 \sum_{k=1}^{N} v_c^{1/2} \phi_k \left(\mathbb{1}_{\mathcal{H}_1} - \gamma_{0,N}^0 \right) \left(\frac{h_1 - \varepsilon_k}{\omega^2 + (h_1 - \varepsilon_k)^2} \right) \left(\mathbb{1}_{\mathcal{H}_1} - \gamma_{0,N}^0 \right) \phi_k v_c^{1/2}. \qquad (84)$$

In particular, for all $\omega \in \mathbb{R}_\omega$, the operator $\widetilde{P_{\mathrm{sym}}^0}(\mathrm{i}\omega)$ is a negative, self-adjoint bounded operator on $\mathcal{H}_1$ satisfying $\widetilde{P_{\mathrm{sym}}^0}(-\mathrm{i}\omega) = \widetilde{P_{\mathrm{sym}}^0}(\mathrm{i}\omega)$. In addition, the function $\omega \mapsto \widetilde{P_{\mathrm{sym}}^0}(\mathrm{i}\omega)$ is analytic from $\mathbb{R}_\omega$ to $\mathcal{S}(\mathcal{H}_1)$, and is in $L^p(\mathbb{R}_\omega, \mathcal{S}(\mathcal{H}_1))$ for all $p > 1$. For any $f \in \mathcal{H}_1$, the function $\omega \mapsto \left\langle f \middle| \widetilde{P_{\mathrm{sym}}^0}(\mathrm{i}\omega) \middle| f \right\rangle$ is non-positive, in $L^1(\mathbb{R}_\omega)$, and

$$\int_{-\infty}^{+\infty} \left\langle f \middle| \widetilde{P_{\mathrm{sym}}^0}(\mathrm{i}\omega) \middle| f \right\rangle \mathrm{d}\omega = -2\pi \left\langle f \middle| v_c^{1/2} \left(\left(\mathbb{1}_{\mathcal{H}_1} - \gamma_{0,N}^0 \right) \odot \gamma_{0,N}^0 \right) v_c^{1/2} \middle| f \right\rangle$$

$$= -2\pi \left\langle f \middle| \sum_{k=1}^{N} v_c^{1/2} \phi_k \left(\mathbb{1}_{\mathcal{H}_1} - \gamma_{0,N}^0 \right) \phi_k v_c^{1/2} \middle| f \right\rangle. \qquad (85)$$

Finally, there exists a constant $C \in \mathbb{R}^+$ such that

$$\forall \omega \in \mathbb{R}_\omega, \quad 0 \leqslant -\widetilde{P_{\mathrm{sym}}^0}(\mathrm{i}\omega) \leqslant \frac{C}{(\omega^2 + 1)^{1/2}} \left(v_c^{1/2} \rho_{0,N}^0 v_c^{1/2} \right), \qquad (86)$$

where $\rho_{0,N}^0$ is the multiplication operator by the (real-valued) function $\rho_{0,N}^0$, the latter operator being bounded from $\mathcal{C}'$ to $\mathcal{C}$.

The sum-rule for the operator $\widetilde{P^0}$. We end this section with the sum-rule for the operator $\widetilde{P^0} = v_c^{-1/2} \widetilde{P_{\mathrm{sym}}^0} v_c^{-1/2}$, which goes from $\mathcal{C}'$ to $\mathcal{C}$. We postpone the proof until Section 6.17.

Theorem 60. *The operator $2 \sum_{k=1}^{N} \phi_k (\mathbb{1}_{\mathcal{H}_1} - \gamma_{0,N}^0)(h_1 - \varepsilon_k)\phi_k$ is bounded from $\mathcal{C}'$ to $\mathcal{C}$, and it holds*

$$2 \sum_{k=1}^{N} \phi_k (\mathbb{1}_{\mathcal{H}_1} - \gamma_{0,N}^0)(h_1 - \varepsilon_k)\phi_k = \mathrm{div}\,(\rho_{0,N}^0 \nabla \cdot).$$

Moreover, the following weak-convergence holds:

$$\forall (f, g) \in \mathcal{C}' \times \mathcal{C}', \quad \lim_{\omega \to \pm\infty} \left\langle \overline{f}, -\omega^2 \widetilde{P^0}(\mathrm{i}\omega) g \right\rangle_{\mathcal{C}', \mathcal{C}} = \left\langle \overline{f}, -\mathrm{div}\,\left(\rho_{0,N}^0 \nabla g \right) \right\rangle_{\mathcal{C}', \mathcal{C}} = \int_{\mathbb{R}^3} \rho_{0,N}^0 \overline{\nabla f} \cdot \nabla g.$$

Finally, for all $g \in \mathcal{C}'$ such that $\Delta g \in L^2(\mathbb{R}^3)$, the following strong convergence holds:

$$\lim_{\omega \to \pm\infty} \omega^2 \widetilde{P^0}(\mathrm{i}\omega) g = \mathrm{div}\,\left(\rho_{0,N}^0 \nabla g \right) \quad \text{in } \mathcal{C}.$$

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This sum-rule automatically leads to a sum-rule for the reducible polarizability operator in the random phase approximation χ^0 (see Theorem 67).

4.2.2 The analytical continuation method

In this section, we explain why (74a) can be thought of as a natural reformulation of the usual physical definition (75), and why problems arise with Definition (74a) (see Problem 55). This section also serves as a guideline to understand why (74d) is a natural reformulation of the usual physical definition of Σ^{GW} (see (97) below). In the previous section, we gave the properties of $\widetilde{P^0}$ using the explicit expression of P^0 given in (81). While this approach simplifies the proofs, it somehow hides some structural properties that we highlight in this section.

Recall that $P_{\mathrm{sym}}^0 = P_{\mathrm{sym}}^{0,+} + P_{\mathrm{sym}}^{0,-}$ with

$$P_{\mathrm{sym}}^{0,+}(\tau) = -\mathrm{i}\Theta(\tau)v_c^{1/2}G_{0,\mathrm{p}}(\tau) \odot G_{0,\mathrm{h}}(-\tau)v_c^{1/2}$$

and

$$P_{\mathrm{sym}}^{0,-}(\tau) = -\mathrm{i}\Theta(-\tau)v_c^{1/2}G_{0,\mathrm{h}}(\tau) \,\widetilde{\odot}\, G_{0,\mathrm{p}}(-\tau)v_c^{1/2},$$

where

$$G_{0,\mathrm{p}}(\tau) = -\mathrm{i}\Theta(\tau)A_{0,+}\mathrm{e}^{-\mathrm{i}\tau(H_{0,N+1}-E_{0,N}^0)}A_{0,+}^*, \qquad G_{0,\mathrm{h}}(\tau) = \mathrm{i}\Theta(-\tau)A_{0,-}^*\mathrm{e}^{\mathrm{i}\tau(H_{0,N-1}-E_{0,N}^0)}A_{0,-}.$$

The idea is to use the results of Theorem 24. We first consider $P_{\mathrm{sym}}^{0,+}$, and prove that the hypotheses of Theorem 24 are satisfied. This is given by the following lemma.

Lemma 61. *There exists a constant $C \in \mathbb{R}^+$ such that, for any $f \in \mathcal{H}_1$, it holds $A_{0,-}\left(v_c^{1/2}f\right) \in \mathfrak{S}_2(\mathcal{H}_1)$ with*

$$\left\|A_{0,-}\left(v_c^{1/2}f\right)\right\|_{\mathfrak{S}_2(\mathcal{H}_1)} \leqslant C\|f\|_{\mathcal{H}_1}.$$

Moreover, $H_{0,N+1} - E_{0,N}^0 \geqslant \varepsilon_{N+1}$ and $H_{0,N-1} - E_{0,N}^0 \geqslant -\varepsilon_N$.

Proof. The first point comes from the fact that $A_{0,-}^*A_{0,-} = \gamma_{0,N}^0$ and that $v_c^{1/2}f \in \mathcal{C}' \hookrightarrow L^6$ whenever $f \in \mathcal{H}_1$, together with Lemma 77. $\qquad\square$

In particular, the hypotheses of Theorem 24 are satisfied, and we deduce that for any $\nu' > \varepsilon_N$ and $\nu + \nu' < \varepsilon_{N+1}$,

$$\forall \omega \in \mathbb{R}, \quad \widetilde{P_{\mathrm{sym}}^{0,+}}(\nu + \mathrm{i}\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} v_c^{1/2}\left(\widetilde{G_{0,\mathrm{p}}}\big(\nu + \nu' + \mathrm{i}(\omega + \omega')\big) \odot \widetilde{G_{0,\mathrm{h}}}(\nu' + \mathrm{i}\omega')\right)v_c^{1/2}\mathrm{d}\omega'. \tag{87}$$

We treat $\widetilde{P_{\mathrm{sym}}^{0,-}}$ is a similar way, and find that for any $\nu' < \varepsilon_{N+1}$ and $\nu + \nu' > \varepsilon_N$,

$$\forall \omega \in \mathbb{R}, \quad \widetilde{P_{\mathrm{sym}}^{0,-}}(\nu + \mathrm{i}\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} v_c^{1/2}\left(\widetilde{G_{0,\mathrm{h}}}\big(\nu + \nu' + \mathrm{i}(\omega + \omega')\big) \,\widetilde{\odot}\, \widetilde{G_{0,\mathrm{p}}}(\nu' + \mathrm{i}\omega')\right)v_c^{1/2}\mathrm{d}\omega'. \tag{88}$$

Actually, the kernel-product $\widetilde{\odot}$ in the latter expression can be transformed into the kernel-product $\odot$, thanks to the following lemma, whose proof is given in Section 6.18.

Lemma 62. *For any $\nu' < \varepsilon_{N+1}$, any $\nu + \nu' > \varepsilon_N$ and any $\omega, \omega' \in \mathbb{R}_\omega$,*

$$\widetilde{G_{0,\mathrm{h}}}\big(\nu + \nu' + \mathrm{i}(\omega + \omega')\big) \,\widetilde{\odot}\, \widetilde{G_{0,\mathrm{p}}}(\nu' + \mathrm{i}\omega') = \widetilde{G_{0,\mathrm{h}}}\big(\nu + \nu' + \mathrm{i}(\omega + \omega')\big) \odot \widetilde{G_{0,\mathrm{p}}}(\nu' + \mathrm{i}\omega'),$$

as bounded operators from $\mathcal{C}'$ to $\mathcal{C}$.

We can perform the same type of calculation for $G_{\mathrm{h}} \odot G_{\mathrm{h}}$. Following the proof of Theorem 24, we deduce from $G_{\mathrm{h}}(\tau) \odot G_{\mathrm{h}}(-\tau) = 0$ that, for any $\nu' > \varepsilon_N$ and $\nu + \nu' > \varepsilon_N$,

$$\forall \omega \in \mathbb{R}_\omega, \quad \frac{1}{2\pi} \int_{-\infty}^{+\infty} v_c^{1/2} \left(\widetilde{G_{0,\mathrm{h}}}\big(\nu + \nu' + \mathrm{i}(\omega + \omega')\big) \odot \widetilde{G_{0,\mathrm{h}}}(\nu' + \mathrm{i}\omega') \right) v_c^{1/2} \mathrm{d}\omega' = 0. \tag{89}$$

Similarly, from $G_{\mathrm{p}}(\tau) \odot G_{\mathrm{p}}(-\tau) = 0$, we deduce that, *at least formally*, for any $\nu' < \varepsilon_{N+1}$, and any $\nu + \nu' < \varepsilon_{N+1}$,

$$\forall \omega \in \mathbb{R}_\omega, \quad \frac{1}{2\pi} \int_{-\infty}^{+\infty} v_c^{1/2} \left(\widetilde{G_{0,\mathrm{p}}}\big(\nu + \nu' + \mathrm{i}(\omega + \omega')\big) \odot \widetilde{G_{0,\mathrm{p}}}(\nu' + \mathrm{i}\omega') \right) v_c^{1/2} \mathrm{d}\omega' = 0. \tag{90}$$

Remark 63. *The last equality is formal, in the sense that the integrand $\widetilde{G_{0,\mathrm{p}}} \odot \widetilde{G_{0,\mathrm{p}}}$ is actually not well-defined: it does not define a bounded operator from $\mathcal{C}'$ to $\mathcal{C}$. However, we can proceed as follows. For $\omega \in \mathbb{R}_\omega$, let $\widetilde{P_\sharp^{+,+}}(\mathrm{i}\omega)$ be the operator defined on the core $\mathcal{H}_1 \cap \mathcal{C}$ by*

$$\forall f, g \in \mathcal{H}_1 \cap \mathcal{C}, \quad \left\langle f \left| \widetilde{P_\sharp^{+,+}}(\mathrm{i}\omega) \right| g \right\rangle$$
$$:= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathrm{Tr}_{\mathcal{H}_1} \left[\widetilde{G_{0,\mathrm{p}}}\big(\nu + \nu' + \mathrm{i}(\omega + \omega')\big) \left(v_c^{1/2} g \right) \widetilde{G_{0,\mathrm{p}}}(\nu' + \mathrm{i}\omega') \left(v_c^{1/2} \overline{f} \right) \right] \mathrm{d}\omega'.$$

Noticing that $v_c^{1/2} \overline{f}$ and $v_c^{1/2} g$ are in $\mathcal{H}_1$ since $f, g \in \mathcal{C}$, and reasoning as in the proof of Lemma 62, we can prove that the operator in the trace is indeed trace-class, with

$$\left| \mathrm{Tr}_{\mathcal{H}_1} \left[\widetilde{G_{0,\mathrm{p}}}\big(\nu + \nu' + \mathrm{i}(\omega + \omega')\big) \left(v_c^{1/2} g \right) \widetilde{G_{0,\mathrm{p}}}(\nu' + \mathrm{i}\omega') \left(v_c^{1/2} \overline{f} \right) \right] \right| \leqslant p_\omega(\omega') \|f\|_{\mathcal{C}} \|g\|_{\mathcal{C}},$$

where p_ω is an integrable function independent of f and g. Moreover, following the proof of Theorem 24, we can prove that, as expected,

$$\forall f, g \in \mathcal{H}_1 \cap \mathcal{C}, \quad \left\langle f \left| \widetilde{P_\sharp^{+,+}}(\mathrm{i}\omega) \right| g \right\rangle = 0.$$

The unique continuation on $\mathcal{H}_1$ of $\widetilde{P_\sharp^{+,+}}(\mathrm{i}\omega)$ therefore is the null operator. It is unclear to us how to extend a similar reasoning for a generic class of approximated Green's function $\widetilde{G^{\mathrm{app}}}$.

By gathering (87), (88), (89) and (90), we find that, for any $\nu' \in (\varepsilon_N, \varepsilon_{N+1})$ and $\nu + \nu' \in (\varepsilon_N, \varepsilon_{N+1})$,

$$\forall \omega \in \mathbb{R}_\omega, \quad \widetilde{P_{\mathrm{sym}}^0}(\nu + \mathrm{i}\omega) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} v_c^{1/2} \left(\widetilde{G_0}\big(\nu + \nu' + \mathrm{i}(\omega' + \omega)\big) \odot \widetilde{G_0}(\nu' + \mathrm{i}\omega') \right) v_c^{1/2} \mathrm{d}\omega'.$$

In particular, this equality holds for the particular choice $\nu' = \mu_0$ and $\nu = 0$.

Remark 64. *To summarize the work performed in this section, we transformed the equation*

$$P^0(\mathbf{r}, \mathbf{r}', \tau) := -\mathrm{i} G_0(\mathbf{r}, \mathbf{r}', \tau) G_0(\mathbf{r}', \mathbf{r}, -\tau) \tag{91}$$

into: for any $\nu' \in (\varepsilon_N, \varepsilon_{N+1})$ and $\nu \in (\varepsilon_N - \nu', \varepsilon_{N+1} - \nu')$

$$\widetilde{P^0}(\nu + \mathrm{i}\cdot) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \left(\widetilde{G_0}\big(\nu + \nu' + \mathrm{i}(\omega' + \cdot)\big) \odot \widetilde{G_0}(\nu' + \mathrm{i}\omega') \right) \mathrm{d}\omega'. \tag{92}$$

Note that the manipulations performed in this section to transform (91) into (92) are possible since the two operators involved in the kernel-product (here, both are equal to $\widetilde{G^0}(z)$) are analytic on some common domain $\mathbb{U} \cup \mathbb{L} \cup (a, b)$ with $a < b$ (the presence of a gap is important to deform the contour as in Theorem 24).

4.2.3 The RPA reducible polarizability operator χ^0

In order to calculate the GW approximation of the self-energy, one needs the reducible polariz-ability operator χ, defined in Section 3.3.2. Unfortunally, the expression of χ is not accessible in practice. One needs to approximate this operator. The GW approximation, which amounts to approximating the so-called *vertex function*, provides a natural approximation χ^{GW} of χ: in Equation (74b), χ^{GW} is defined from G^{GW} (see also [11, Equation (103)] or [18, Equations (A.20) and (A.28)]). However, in view of Remark 55, the definition of χ^{GW} is not well-understood math-ematically. In the GW^0 framework, we use the RPA reducible polarizability operator χ^0, which is itself defined in terms of the RPA irreducible polarizability P^0. The GW^0 approximation of the (symmetrized) reducible polarizability operator is usually defined in the frequency domain as

$$\widehat{\chi^0_{\mathrm{sym}}}(\omega) := \left(\mathbb{1}_{\mathcal{H}_1} - \widehat{P^0_{\mathrm{sym}}}(\omega) \right)^{-1} - \mathbb{1}_{\mathcal{H}_1}.$$

The formal analytic continuation of the above definitions is (see [11, Equation (139)])

$$\widetilde{\chi^0_{\mathrm{sym}}}(z) := \left(\mathbb{1}_{\mathcal{H}_1} - \widetilde{P^0_{\mathrm{sym}}}(z) \right)^{-1} - \mathbb{1}_{\mathcal{H}_1}. \tag{93}$$

Note that we use the "tilde" notation in $\widetilde{\chi^0_{\mathrm{sym}}}$, although it is unclear that this operator-valued function is indeed the Laplace transform of some operator-valued function in the time domain. Also, it is *a priori* unclear whether the operators $\mathbb{1}_{\mathcal{H}_1} - \widehat{P^{\mathrm{GW}}_{\mathrm{sym}}}(\omega)$ or $\mathbb{1}_{\mathcal{H}_1} - \widetilde{P^{\mathrm{GW}}_{\mathrm{sym}}}(z)$ are invertible. This is however the case for appropriate values of z, as shown by the following lemma.

Lemma 65. *For $z \in (-(\varepsilon_{N+1} - \varepsilon_N), \varepsilon_{N+1} - \varepsilon_N)$ and $z \in i\mathbb{R}$, the operator $\mathbb{1}_{\mathcal{H}_1} - \widetilde{P^0_{\mathrm{sym}}}(z)$ is invertible.*

This result is a direct consequence of the explicit formula (83) for $\widetilde{P^0}$, which ensures that $\widetilde{P^0_{\mathrm{sym}}}(z)$ is a bounded self-adjoint negative operator for the values of z under consideration. Let us deduce some extra properties of $\widetilde{\chi^0}$.

Lemma 66. *For any $\omega \in \mathbb{R}$, the operator $\widetilde{\chi^0_{\mathrm{sym}}}(i\omega)$ is a bounded, negative, self-adjoint operator on $\mathcal{H}_1$, satisfying $\widetilde{\chi^0_{\mathrm{sym}}}(-i\omega) = \widetilde{\chi^0_{\mathrm{sym}}}(i\omega)$, and such that*

$$\widetilde{P^0_{\mathrm{sym}}}(i\omega) \leqslant \widetilde{\chi^0_{\mathrm{sym}}}(i\omega) \leqslant 0. \tag{94}$$

The function $\omega \mapsto \widetilde{\chi^0_{\mathrm{sym}}}(i\omega)$ is analytic from $\mathbb{R}_\omega$ to $\mathcal{S}(\mathcal{H}_1)$ and is in $L^p(\mathbb{R}_\omega, \mathcal{S}(\mathcal{H}_1))$ for all $p > 1$. Finally, there exists a constant $C \in \mathbb{R}^+$ such that

$$0 \leqslant -\widetilde{\chi^0_{\mathrm{sym}}}(i\omega) \leqslant \frac{C}{(\omega^2 + 1)^{1/2}} \left(v_c^{1/2} \rho^0_{0,N} v_c^{1/2} \right). \tag{95}$$

This result is deduced from the definition (93), the inequality $x \leqslant (1-x)^{-1} - 1 \leqslant 0$ for $x \leqslant 0$, and Proposition 59.

Sum-rule for $\widetilde{\chi^0}$. From the sum-rule stated in Theorem 60, we readily deduce the sum-rule for $\widetilde{\chi^0} := v_c^{-1/2} \widetilde{\chi^0_{\mathrm{sym}}} v_c^{-1/2}$, which is a bounded operator from $\mathcal{C}'$ to $\mathcal{C}$. Indeed, from the equality $(1-x)^{-1} - 1 = x + x^2(1-x)^{-1}$, we obtain

$$\forall \omega \in \mathbb{R}_\omega, \quad \widetilde{\chi^0_{\mathrm{sym}}}(i\omega) = \widetilde{P^0_{\mathrm{sym}}}(i\omega) + \left(\widetilde{P^0_{\mathrm{sym}}}(i\omega) \right)^2 \left(\mathbb{1}_{\mathcal{H}_1} - \widetilde{P^0_{\mathrm{sym}}}(i\omega) \right)^{-1}.$$

In particular,

$$\forall \omega \in \mathbb{R}_\omega, \quad \omega^2 \widetilde{\chi^0}(i\omega) = \omega^2 \widetilde{P^0}(i\omega) + \frac{1}{\omega^2} \left(\omega^2 \widetilde{P^0}(i\omega) \right) \left(v_c^{1/2} \left(\mathbb{1}_{\mathcal{H}_1} - \widetilde{P^0_{\mathrm{sym}}}(i\omega) \right)^{-1} v_c^{1/2} \right) \left(\omega^2 \widetilde{P^0}(i\omega) \right).$$

This shows that the asymptotic behavior of $\widetilde{\chi^0}(\mathrm{i}\omega)$ is, at dominant order, the same as for $\widetilde{P^0}(\mathrm{i}\omega)$. Taking the limit $\omega \to \pm\infty$ leads to a theorem similar to Theorem 60, whose proof is skipped here for the sake of brevity.

Theorem 67. *The following weak-convergence holds:*

$$\forall(f,g) \in \mathcal{C}' \times \mathcal{C}', \quad \lim_{\omega\to\pm\infty} \left\langle \overline{f}, -\omega^2\widetilde{\chi^0}(\mathrm{i}\omega)g \right\rangle_{\mathcal{C}',\mathcal{C}} = \left\langle \overline{f}, -\mathrm{div}\left(\rho^0_{0,N}\nabla g\right)\right\rangle_{\mathcal{C}',\mathcal{C}} = \int_{\mathbb{R}^3}\rho^0_{0,N}\overline{\nabla f}\cdot\nabla g.$$

For all $g \in \mathcal{C}'$ such that $\Delta g \in L^2(\mathbb{R}^3)$, the following strong convergence holds:

$$\lim_{\omega\to\pm\infty}\omega^2\widetilde{\chi^0}(\mathrm{i}\omega)g = \mathrm{div}\left(\rho^0_{0,N}\nabla g\right) \quad \text{in } \mathcal{C}.$$

By comparing Theorems 67 and 46, we see why using (71) instead of (70) for the definition of h_1 may lead to better approximations, since $\rho^0_{0,N} = \rho^0_N$ in this case, so that the GW approximation χ^{GW} of χ becomes exact in the high imaginary frequency domain.

Theorem 67 is useful for the design of the so-called *Plasmon-Pole models* (PPM) [22, 47, 16, 10]. Since the definition (93) requires the computation of a resolvent, the calculation of $\widetilde{\chi^0}(z)$ is numerically very expensive in practice. Some authors suggested to approximate $\widetilde{\chi^0}$ by an operator $\widetilde{\chi^{\mathrm{PPM}}}$ which is computationally less expensive. In practice, $\widetilde{\chi^{\mathrm{PPM}}}$ has a prescribed functional form, with adjustable parameters. Different approaches are taken in order to tune these parameters, and the previous sum-rule provides a standard way to fit some of them. This is done for instance in the PPM by Hybersten and Louie [22] and in the PPM by Engel and Farid [10]. In the later article, the authors extensively comment on the fact that this sum-rule is an important requirement to be satisfied for a PPM.

4.2.4 The RPA dynamically screened operator W^0

From the approximation χ^0 of χ, we directly deduce the approximation W^0 of W. Following the path taken in Section 3.3.4, we define

$$\widetilde{W^0}(z) := v_c + \widetilde{W^0_c}(z) \quad \text{with} \quad \widetilde{W^0_c}(z) := v_c^{1/2}\widetilde{\chi^0_{\mathrm{sym}}}(z)v_c^{1/2}. \tag{96}$$

This operator, when well-defined (say on the gap $(-(\varepsilon_{N+1} - \varepsilon_N), \varepsilon_{N+1} - \varepsilon_N)$ or on the imaginary axis $\mathrm{i}\mathbb{R}$) is a bounded operator from $\mathcal{C}$ to $\mathcal{C}'$. The properties of $\widetilde{W^0}$ are directly deduced from the ones of $\widetilde{\chi^0_{\mathrm{sym}}}$, so we do not repeat them here for brevity.

4.3 A mathematical study of the GW^0 approximation

4.3.1 The $\mathrm{G}_0\mathrm{W}^0$ approximation of the self-energy

In this section, we study the $\mathrm{G}_0\mathrm{W}^0$ approximation as a preliminary step to the study of the self-consistent GW^0 approximation. This will help us understand some technical points to address in the analysis of the GW^0 method.

The $\mathrm{G}_0\mathrm{W}^0$ approximation of the self-energy operator is formally defined as

$$\Sigma^{00}(\mathbf{r},\mathbf{r}',\tau) := \mathrm{i}G_0(\mathbf{r},\mathbf{r}',\tau)W^0(\mathbf{r},\mathbf{r}',-\tau^+). \tag{97}$$

Here, G_0 represents the Green's function of the non-interacting system introduced in Definition 47, and W^0 is the random phase approximation of the dynamically screened operator defined in Section 4.2.4. Already one difficulty arises: in Section 4.2.4, we only defined the function $\widetilde{W^0}(z)$ on the complex frequency domain, but we did not define some operator-valued function on the time-domain. In this section, we assume that the function $\widetilde{W^0}(z)$ is indeed the Laplace transform

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of some operator $W^0(\tau)$. This will allow us to transform (97) into a formally equivalent definition that only involves $\widetilde{W^0}$. The resulting definition will be our starting point for the GW^0 approximation.

With the kernel-product defined in Section 2.4.1, the definition (97) can be recast as

$$\Sigma^{00}(\tau) = \mathrm{i}G_0(\tau^-) \odot W^0(-\tau).$$

In view of the decomposition provided in (96), it is natural to split Σ^{00} into an exchange part Σ_x^{00} and a correlation part Σ_c^{00} (the terminology is motivated below):

$$\Sigma^{00} = \Sigma_x^{00} + \Sigma_c^{00} \quad \text{with} \quad \Sigma_x^{00}(\tau) = \mathrm{i}G_{0,\mathrm{h}}(0^-) \odot v_c \delta_0(\tau) \quad \text{and} \quad \Sigma_c^{00}(\tau) = \mathrm{i}G_0(\tau) \odot W_c(-\tau).$$

Let us first consider the exchange part. As $\mathrm{i}G_{0,\mathrm{h}}(0^-) = -\gamma_{0,N}^0$, we obtain

$$\Sigma_x^{00}(\tau) = K_x \delta_0(\tau), \tag{98}$$

where K_x is the integral operator on $\mathcal{H}_1$ with kernel

$$K_x(\mathbf{r}, \mathbf{r}') := -\frac{\gamma_{0,N}^0(\mathbf{r}, \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}. \tag{99}$$

We recover the usual Fock exchange operator associated with $\gamma_{0,N}^0$, which justifies the terminology "exchange part" for Σ_x^{00}. Let us now consider the correlation part. Observing that

- $\widetilde{G_0}$ is analytic on $\mathbb{U} \cup \mathbb{L} \cup (\varepsilon_N, \varepsilon_{N+1})$ (hence has a gap around μ_0) ;

- $\widetilde{W^0}$ is analytic on $\mathbb{U} \cup \mathbb{L} \cup (-(\varepsilon_{N+1} - \varepsilon_N), \varepsilon_{N+1} - \varepsilon_N)$ (hence has a gap around 0),

we can use the same ideas as in Section 4.2.2. *By analogy* with Remark 64, we recast the physical definition of $\widetilde{\Sigma^{00}}$ in (97) in a *formally equivalent* definition in the complex frequency plane. This reformulation was first given by Rojas, Godby and Needs [36] (see also [34]), and is now known as the "contour deformation" technique.

Definition 68 (G$_0$W^0 approximation of the self-energy). *The exchange part of the self-energy in the G_0W^0 approximation is defined in the complex frequency domain by*

$$\forall z \in \mathbb{C}, \qquad \widetilde{\Sigma_x^{00}}(z) = K_x,$$

while the correlation part is defined, for $\nu' \in (-(\varepsilon_{N+1} - \varepsilon_N), \varepsilon_{N+1} - \varepsilon_N)$ and $\nu + \nu' \in (\varepsilon_N, \varepsilon_{N+1})$ by

$$\forall \omega \in \mathbb{R}_\omega, \quad \widetilde{\Sigma_c^{00}}(\nu + \mathrm{i}\omega) = -\frac{1}{2\pi} \int_{-\infty}^{+\infty} \widetilde{G_0}\left(\nu + \nu' + \mathrm{i}(\omega + \omega')\right) \odot \widetilde{W_c^0}(\nu' + \mathrm{i}\omega') \, \mathrm{d}\omega.$$

The fact that the above quantity is independent of the choice of ν' comes from the analyticity of the integrand on the region of interest. In practice, we will focus on the case $\nu' = 0$ and $\nu = \mu_0$, and therefore consider the function $\mathbb{R}_\omega \ni \omega \mapsto \widetilde{\Sigma_0^{00}}(\mu_0 + \mathrm{i}\omega)$ defined by

$$\forall \omega \in \mathbb{R}_\omega, \quad \widetilde{\Sigma_c^{00}}(\mu_0 + \mathrm{i}\omega) = -\frac{1}{2\pi} \int_{-\infty}^{+\infty} \widetilde{G_0}\left(\mu_0 + \mathrm{i}(\omega + \omega')\right) \odot \widetilde{W_c^0}(\mathrm{i}\omega') \, \mathrm{d}\omega. \tag{100}$$

The next proposition shows that the above definition makes sense.

Proposition 69. *The operator K_x arising in the exchange part Σ_c^{00} of the self-energy is a negative Hilbert-Schmidt operator on $\mathcal{H}_1$. Furthermore, for any $\omega \in \mathbb{R}_\omega$, the operator $\widetilde{\Sigma_c^{00}}(\mu_0 + \mathrm{i}\omega)$ is a bounded operator on $\mathcal{H}_1$, and satisfies $\widetilde{\Sigma_c^{00}}(\mu_0 - \mathrm{i}\omega) = \widetilde{\Sigma_c^{00}}(\mu_0 + \mathrm{i}\omega)^*$. The function $\omega \mapsto \widetilde{\Sigma_c^{00}}(\mu_0 + \mathrm{i}\omega)$ is analytic from $\mathbb{R}_\omega$ to $\mathcal{B}(\mathcal{H}_1)$ and is in $L^p(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$ for all $p > 1$.*

The first statements of Proposition 69 can be seen as a special case of Proposition 73, while the symmetry property for the adjoint and the L^p integrability follow from the properties of $\widetilde{G^0}$ and $\widetilde{W_c^0}$.

4.3.2 Well-posedness of the GW^0 approximation in the perturbative regime.

We finally study the GW^0 approximation. Following our definition (100) of the $\mathrm{G}_0\mathrm{W}^0$ approximation of the self-energy, we recast the GW^0 equation as follows.

Definition 70 (The GW^0 problem on the imaginary axis in the frequency domain).
Find $G^{\mathrm{GW}^0} \in L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$ solution to the system

$$(\mathrm{GW}^0) \quad \begin{cases} \widetilde{\Sigma^{\mathrm{GW}^0}}(\mu_0 + \mathrm{i}\omega) = K_x - \dfrac{1}{2\pi} \displaystyle\int_{-\infty}^{+\infty} \widetilde{G^{\mathrm{GW}^0}}\big(\mu_0 + \mathrm{i}(\omega + \omega')\big) \odot \widetilde{W_c^0}(\mathrm{i}\omega')\,\mathrm{d}\omega', \\[2mm] \widetilde{G^{\mathrm{GW}^0}}(\mu_0 + \mathrm{i}\omega) = \Big[\mu_0 + \mathrm{i}\omega - \Big(h_1 + \widetilde{\Sigma^{\mathrm{GW}^0}}(\mu_0 + \mathrm{i}\omega)\Big)\Big]^{-1}, \end{cases}$$

where h_1 is the one-body mean-field Hamiltonian defined in (70) and K_x is the exchange operator defined by (67)-(99).

Remark 71. *We are looking for a solution in $L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$. Note that the true Green's function $\widetilde{G}(\mu + \mathrm{i}\cdot)$ is in $L^p(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$ for all $p > 1$ (in particular for $p = \infty$). We chose to work with $L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1)$ for simplicity, but it is possible to work with other spaces $L^p(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$ with $p > 1$.*

Since this problem seems quite difficult to study mathematically, we will only study it in a perturbative regime. More specifically, seeing Σ^{GW} as a correction term (see the discussion after Definition 52), we propose to study the following problem.

Definition 72 (The GW^0_λ problem on the imaginary axis on the frequency domain).
Find $G^{\mathrm{GW}^0_\lambda} \in L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$ solution of the system

$$(\mathrm{GW}^0_\lambda) \quad \begin{cases} \widetilde{\Sigma^{\mathrm{GW}^0_\lambda}}(\mu_0 + \mathrm{i}\omega) = K_x - \dfrac{1}{2\pi} \displaystyle\int_{-\infty}^{+\infty} \widetilde{G^{\mathrm{GW}^0_\lambda}}\big(\mu_0 + \mathrm{i}(\omega + \omega')\big) \odot \widetilde{W_c^0}(\mathrm{i}\omega')\,\mathrm{d}\omega' \\[2mm] \widetilde{G^{\mathrm{GW}^0_\lambda}}(\mu_0 + \mathrm{i}\omega) = \Big[\mu_0 + \mathrm{i}\omega - \Big(h_1 + \lambda\widetilde{\Sigma^{\mathrm{GW}^0_\lambda}}(\mu_0 + \mathrm{i}\omega)\Big)\Big]^{-1}. \end{cases} \tag{101}$$

According to (69), the unique solution for $\lambda = 0$ is the Green's function for the non interacting system $\widetilde{G^{\mathrm{GW}^0_{\lambda=0}}} = \widetilde{G_0}$. This fact will allow us to treat the equation perturbatively. The exact GW^0 equations correspond to the case $\lambda = 1$. Of course, several other choices of perturbation can be used. For instance, we can put the parameter λ in front of the correlation part of the self-energy only. This amounts to considering the Hartree-Fock Hamiltonian as the reference Hamiltonian (instead of the Hartree Hamiltonian). The theory that we develop here can be straightforwardly generalized to such other cases.

It is convenient for the mathematical analysis to introduce the functionals $\mathfrak{s}$ and $\mathfrak{g}$ respectively defined as

$$\begin{array}{rcl} \mathfrak{s}: \quad L^2(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1)) & \to & L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1)) \\ \widetilde{G^{\mathrm{app}}}(\mu_0 + \mathrm{i}\cdot) & \mapsto & \mathfrak{s}\Big[\widetilde{G^{\mathrm{app}}}\Big](\mu_0 + \mathrm{i}\cdot) := K_x - \dfrac{1}{2\pi} \displaystyle\int_{-\infty}^{+\infty} \widetilde{G^{\mathrm{app}}}(\mu_0 + \mathrm{i}(\cdot + \omega')) \odot \widetilde{W_c^0}(\mathrm{i}\omega')\,\mathrm{d}\omega', \end{array}$$

and

$$\begin{array}{rcl} \mathfrak{g}_\lambda: \quad L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1)) & \to & L^2(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1)) \\ \widetilde{\Sigma^{\mathrm{app}}}(\mu_0 + \mathrm{i}\cdot) & \mapsto & \mathfrak{g}\Big[\widetilde{\Sigma^{\mathrm{app}}}\Big](\mu_0 + \mathrm{i}\cdot) := \Big[\mu_0 + \mathrm{i}\cdot - \Big(h_1 + \lambda\widetilde{\Sigma^{\mathrm{app}}}(\mu_0 + \mathrm{i}\cdot)\Big)\Big]^{-1}. \end{array}$$

With this notation, $\widetilde{G^{\mathrm{GW}^0_\lambda}}$ is a solution of the GW^0_λ equations (101) if and only if it is a fixed-point of $\mathfrak{g}_\lambda \circ \mathfrak{s}$. The fact that these maps are indeed well-defined is proved in the following proposition (see Section 6.19 for the proof).

Proposition 73. *The operator $\mathfrak{s}$ is a bounded linear operator from $L^2(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$ to $L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$. On the other hand, for all $M > 0$, there exists $\lambda_M > 0$ and $C_M \in \mathbb{R}^+$ such that for all $0 \leqslant \lambda < \lambda_M$, and all $\widetilde{\Sigma^{\mathrm{app}}}$ such that $\left\| \widetilde{\Sigma^{\mathrm{app}}}(\mu_0 + \mathrm{i}\cdot) \right\|_{L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))} \leqslant M$, the function $\mathfrak{g}_\lambda[\Sigma^{\mathrm{app}}](\mu_0 + \mathrm{i}\cdot)$ is well-defined as an element of $L^2(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1)) \cap L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$, with*

$$\left\| \mathfrak{g}_\lambda \left[\widetilde{\Sigma^{\mathrm{app}}} \right] (\mu_0 + \mathrm{i}\cdot) \right\|_{L^2(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))} + \left\| \mathfrak{g}_\lambda \left[\widetilde{\Sigma^{\mathrm{app}}} \right] (\mu_0 + \mathrm{i}\cdot) \right\|_{L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))} \leqslant C_M.$$

Moreover, for all $\widetilde{\Sigma_1^{\mathrm{app}}}, \widetilde{\Sigma_2^{\mathrm{app}}} \in L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$ such that $\left\| \widetilde{\Sigma_j^{\mathrm{app}}}(\mu_0 + \mathrm{i}\cdot) \right\|_{L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))} \leqslant M$ for $1 \leqslant j \leqslant 2$,

$$\mathfrak{g}_\lambda \left[\widetilde{\Sigma_1^{\mathrm{app}}} \right] - \mathfrak{g}_\lambda \left[\widetilde{\Sigma_2^{\mathrm{app}}} \right] = \lambda \mathfrak{g}_\lambda \left[\widetilde{\Sigma_1^{\mathrm{app}}} \right] \left(\widetilde{\Sigma_2^{\mathrm{app}}} - \widetilde{\Sigma_1^{\mathrm{app}}} \right) \mathfrak{g}_\lambda \left[\widetilde{\Sigma_2^{\mathrm{app}}} \right]. \tag{102}$$

To prove the existence of a fixed-point for $\mathfrak{g}_\lambda \circ \mathfrak{s}$, we rely on Picard's fixed-point theorem. Since the solution of the $\mathrm{GW}^0_{\lambda=0}$ equations (101) for $\lambda = 0$ is $\widetilde{G_0}$, we are lead to introduce, for $r > 0$, the (closed) ball

$$\mathfrak{B}\left(\widetilde{G_0}, r \right) = \left\{ \widetilde{G^{\mathrm{app}}}(\mu_0 + \mathrm{i}\cdot) \in L^2(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1)), \ \left\| \widetilde{G^{\mathrm{app}}}(\mu_0 + \mathrm{i}\cdot) - \widetilde{G_0}(\mu_0 + \mathrm{i}\cdot) \right\|_{L^2(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))} \leqslant r \right\}.$$

The existence of a fixed-point is given by the following theorem (see Section 6.20 for the proof).

Theorem 74. *There exists $\lambda_* > 0$ and $r > 0$ such that, for all $0 \leqslant \lambda \leqslant \lambda_*$, there exists a unique element $\widetilde{G^{\mathrm{GW}^0_\lambda}} \in \mathfrak{B}\left(\widetilde{G_0}, r \right)$ solution to the GW^0_λ equations (101), or equivalently to the fixed point equation*

$$\widetilde{G^{\mathrm{GW}^0_\lambda}} = \mathfrak{g}_\lambda \circ \mathfrak{s} \left(\widetilde{G^{\mathrm{GW}^0_\lambda}} \right).$$

In addition, for all $\omega \in \mathbb{R}_\omega$, $\widetilde{G^{\mathrm{GW}^0_\lambda}}(\mu_0 + \mathrm{i}\omega)$ is an invertible operator, and

$$\left\| \left(\widetilde{G^{\mathrm{GW}^0_\lambda}}(\mu_0 + \mathrm{i}\cdot) \right)^{-1} - \left(\widetilde{G_0}(\mu_0 + \mathrm{i}\cdot) \right)^{-1} \right\|_{L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))} < \infty. \tag{103}$$

Finally, the iterative sequence $(\mathfrak{g}_\lambda \circ \mathfrak{s})^k \left[\widetilde{G_0} \right]$ converges to $\widetilde{G^{\mathrm{GW}^0_\lambda}}$, and there exists $0 \leqslant \alpha < 1$ and $C \in \mathbb{R}^+$ such that

$$\left\| \left(\widetilde{G^{\mathrm{GW}^0_\lambda}} - (\mathfrak{g}_\lambda \circ \mathfrak{s})^k \left[\widetilde{G_0} \right] \right) (\mu_0 + \mathrm{i}\cdot) \right\|_{L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))} \leqslant C\alpha^k.$$

Remark 75. *It is not difficult to deduce from (103) that the function $\omega \mapsto \widetilde{G^{\mathrm{GW}^0_\lambda}}(\mu + \mathrm{i}\omega)$ is actually in $L^p(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$, for all $p > 1$.*

5 Conclusion

This article is, to our knowledge, the first attempt to formalize with full mathematical rigor the GW theory for finite molecular systems derived by Hedin in his seminal work published in 1965 [18]. In Section 3, we have provided a mathematical definition of some one-body operators arriving in many-body perturbation theory for electronic systems, namely the one-body Green's function G, the spectral function $\mathcal{A}$, the reducible polarizability operator χ, the dynamically screened interaction operator W, and the self-energy operator Σ.

In Section 4, we have worked out a mathematically consistent formulation of the GW^0 approximation of the GW equations, and we have proved that the GW^0 model has a solution in a perturbation regime. As a by-product, we have also shown that the widely used $\mathrm{G_0W}^0$ approximation of the self-energy makes perfect mathematical sense.

6 Proofs

6.1 Proof of Lemma 3

Let $s > 1/2$. For $f \in L^\infty(\mathbb{R}_\tau)$ and $\widehat{\varphi} \in \mathscr{S}(\mathbb{R}_\omega)$,

$$
\left| \langle \mathcal{F}_T f, \widehat{\varphi} \rangle_{\mathscr{S}', \mathscr{S}} \right| = \left| \langle f, \mathcal{F}_T \widehat{\varphi} \rangle_{\mathscr{S}', \mathscr{S}} \right| = 2\pi \left| \int_{\mathbb{R}} f(-\tau)(\mathcal{F}_T^{-1} \widehat{\varphi})(\tau) \, d\tau \right|
$$

$$
= 2\pi \left| \int_{\mathbb{R}} \frac{f(-\tau)}{(1+\tau^2)^{s/2}} (1+\tau^2)^{s/2} (\mathcal{F}_T^{-1} \widehat{\varphi})(\tau) \, d\tau \right| \leqslant C_s \|f\|_{L^\infty} \|\widehat{\varphi}\|_{H^s},
$$

where we have used the Cauchy-Schwarz inequality in the last step. By density, $\mathcal{F}_T f$ can be extended to a linear form on $H^s(\mathbb{R})$. The equality case $\|\mathcal{F}_T f\|_{H^{-s}} = C_s \|f\|_{L^\infty}$ is obtained for constant functions.

6.2 Proof of Theorem 10

Proof of (i). The analyticity of $\widetilde{g}$ directly follows from the results of [38, Chapter VIII].

Proof of (ii). Let $s > 1/2$, and consider $\varphi \in \mathscr{S}(\mathbb{R})$. Relying on the fact that $\widetilde{g}(\cdot + i\eta)$ can be seen as the Fourier transform of $\tau \mapsto g(\tau) e^{-\eta\tau}$, we obtain

$$
\langle \widetilde{g}(\cdot + i\eta), \varphi \rangle_{H^{-s}, H^s} - \langle \widehat{g}, \varphi \rangle_{H^{-s}, H^s} = \langle g \, e^{-\eta\tau}, \widehat{\varphi} \rangle_{\mathscr{S}', \mathscr{S}} - \langle g, \widehat{\varphi} \rangle_{\mathscr{S}', \mathscr{S}}
$$

$$
= \int_0^\infty \left(\frac{g(\tau)}{(1+\tau^2)^{s/2}} \right) (1+\tau^2)^{s/2} \widehat{\varphi}(\tau) \left(e^{-\eta\tau} - 1 \right) d\tau, \tag{104}
$$

where the integral makes sense since $\tau \mapsto g(\tau)(1+\tau^2)^{-s/2}$ and $\tau \mapsto (1+\tau^2)^{s/2}\widehat{\varphi}(\tau)$ are in $L^2(\mathbb{R})$. It is then possible to extend the above formula to any $\varphi \in H^s(\mathbb{R})$. Moreover, by the Cauchy-Schwarz inequality,

$$
\left| \langle \widetilde{g}(\cdot + i\eta), \varphi \rangle_{H^{-s}, H^s} - \langle \widehat{g}, \varphi \rangle_{H^{-s}, H^s} \right| \leqslant I_{\eta, s} \|\varphi\|_{H^s} \|g\|_{L^\infty},
$$

where

$$
I_{\eta, s} = \left(2\pi \int_0^{+\infty} \frac{(1 - e^{-\eta\tau})^2}{(1+\tau^2)^s} \, d\tau \right)^{1/2} < \infty.
$$

Therefore, $\|\widetilde{g}(\cdot + i\eta) - \widehat{g}\|_{H^{-s}} \leqslant \|g\|_{L^\infty} I_{\eta, s}$. By dominated convergence, $I_{\eta, s} \to 0$ as $\eta \to 0^+$, which allows us to conclude to the strong convergence of $\widetilde{g}(\cdot + i\eta)$ to $\widehat{g}$ in $H^{-s}(\mathbb{R}_\omega)$.

A similar computation shows that, for $0 < \eta_1 \leqslant \eta_2$ and $s \in \mathbb{R}$,

$$
\|\widetilde{g}(\cdot + i\eta_1) - \widetilde{g}(\cdot + i\eta_2)\|_{H^s} \leqslant \|g\|_{L^\infty} \left(2\pi \int_0^{+\infty} e^{-2\eta_1\tau} \left(1 - e^{-(\eta_2-\eta_1)\tau} \right)^2 (1+\tau^2)^s \, d\tau \right)^{1/2},
$$

where we crucially use that $\eta_1 > 0$ to ensure the convergence of the time integral when $s > -1/2$. The right-hand side goes to 0 as η_2 goes to η_1 by dominated convergence. This allows one to conclude to the continuity of $\eta \mapsto \widetilde{g}(\cdot + i\eta)$ from $(0, +\infty)$ to $H^s(\mathbb{R})$. When $s < -1/2$, it is possible to pass to the limit $\eta_1 \to 0$ and obtain the uniform continuity from $[0, +\infty)$ to $H^s(\mathbb{R})$.

Proof of (iii). We follow the approach used in [43] for instance. Fix $z_0 \in \mathbb{U}$, and consider, for $R > 0$ and $0 < \alpha \leqslant \text{Im}(z_0)/2$, the oriented contour $\mathscr{C}$ in the complex plane composed of the semi-circle $i\alpha + Re^{i\theta}$ for $0 \leqslant \theta \leqslant \pi$ and the line $i\alpha + \omega$ for $-R \leqslant \omega \leqslant R$. The value R is taken sufficiently large for z_0 to be inside the domain encircled by the contour (see Figure 5).

By Cauchy's residue theorem,

$$
\widetilde{g}(z_0) = \frac{1}{2i\pi} \oint_{\mathscr{C}} \frac{\widetilde{g}(z)}{z - z_0} \, dz = \frac{1}{2i\pi} \int_{-R}^{R} \frac{\widetilde{g}(\omega + i\alpha)}{\omega + i\alpha - z_0} \, d\omega + \frac{1}{2\pi} \int_0^{\pi} \widetilde{g}(i\alpha + Re^{i\theta}) \frac{Re^{i\theta}}{Re^{i\theta} + i\alpha - z_0} \, d\theta. \tag{105}
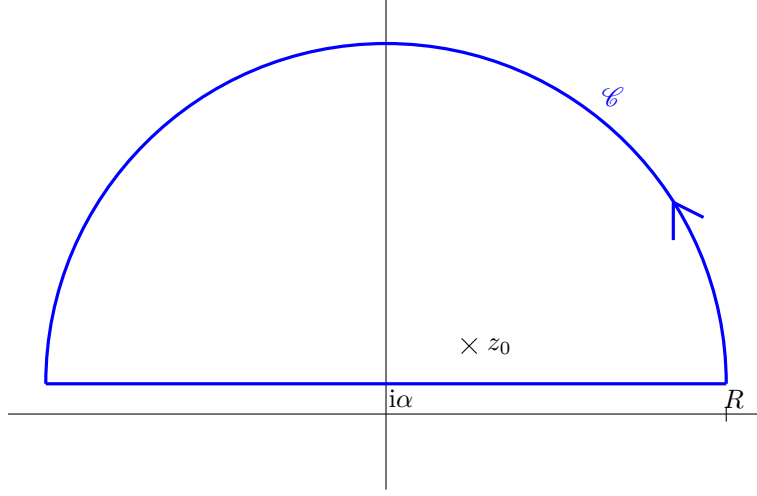$$

Figure 5: The contour $\mathscr{C}$ used in the proof of (iii).

Now, for $z \in \mathbb{U}$,

$$|\widetilde{g}(z)| \leqslant \frac{\|g\|_{L^\infty}}{\operatorname{Im}(z)},$$

so that

$$\left| \int_0^\pi \widetilde{g}(\mathrm{i}\alpha + R\mathrm{e}^{\mathrm{i}\theta}) \frac{R\mathrm{e}^{\mathrm{i}\theta}}{R\mathrm{e}^{\mathrm{i}\theta} + \mathrm{i}\alpha - z_0} \, \mathrm{d}\theta \right| \leqslant \|g\|_{L^\infty} \int_0^\pi \frac{R}{|\alpha + R\sin\theta| \, |R\mathrm{e}^{\mathrm{i}\theta} + \mathrm{i}\alpha - z_0|} \, \mathrm{d}\theta,$$

which, by dominated convergence, converges to 0 as $R \to +\infty$ when α is fixed. On the other hand, $\widetilde{g}(\cdot + \mathrm{i}\alpha)$ belongs to $L^2(\mathbb{R}_\omega)$, while $(\cdot + \mathrm{i}\alpha - z_0)^{-1}$ is in $H^1(\mathbb{R}_\omega)$, since $\mathrm{i}\alpha - z_0$ has a non-zero imaginary part. Therefore, the limit $R \to +\infty$ can be taken in the first integral on the right-hand side of (105), which leads to

$$\widetilde{g}(z_0) = \frac{1}{2\mathrm{i}\pi} \int_{-\infty}^{+\infty} \frac{\widetilde{g}(\omega + \mathrm{i}\alpha)}{\omega + \mathrm{i}\alpha - z_0} \, \mathrm{d}\omega = \frac{1}{2\mathrm{i}\pi} \left\langle \widetilde{g}(\cdot + \mathrm{i}\alpha), (\cdot + \mathrm{i}\alpha - z_0)^{-1} \right\rangle_{H^{-1}, H^1}.$$

The conclusion now follows from the strong convergences of $(\cdot + \mathrm{i}\alpha - z_0)^{-1}$ to $(\cdot - z_0)^{-1}$ in $H^1(\mathbb{R}_\omega)$ and of $\widetilde{g}(\cdot + \mathrm{i}\alpha)$ to $\widehat{g}$ in $H^{-1}(\mathbb{R}_\omega)$ as $\alpha \to 0$.

Proof of (iv). Let φ be a real-valued function in $\mathscr{S}(\mathbb{R}_\omega)$. From (12), we get

$$\int_{\mathbb{R}} \widetilde{g}(\omega + \mathrm{i}\eta)\varphi(\omega) \, \mathrm{d}\omega = \frac{1}{2\mathrm{i}\pi} \int_{\mathbb{R}} \left\langle \widehat{g}, (\cdot - \omega - \mathrm{i}\eta)^{-1} \right\rangle_{H^{-1}, H^1} \varphi(\omega) \, \mathrm{d}\omega.$$

Taking the real parts of both sides, we obtain

$$\begin{aligned}
\int_{\mathbb{R}} &\operatorname{Re}\left(\widetilde{g}(\omega + \mathrm{i}\eta)\right) \varphi(\omega) \, \mathrm{d}\omega \\
&= \frac{1}{2\pi} \int_{\mathbb{R}} \left(\left\langle \operatorname{Im}\widehat{g}, \frac{\cdot - \omega}{(\cdot - \omega)^2 + \eta^2} \right\rangle_{H^{-1}, H^1} + \left\langle \operatorname{Re}\widehat{g}, \frac{\eta}{(\cdot - \omega)^2 + \eta^2} \right\rangle_{H^{-1}, H^1} \right) \varphi(\omega) \, \mathrm{d}\omega.
\end{aligned} \tag{106}$$

Consider now $\phi \in C^\infty(\mathbb{R}^2)$, with support contained in $[-R, R] \times \mathbb{R}$ for some finite $R > 0$. Then, Fubini's theorem for distributions (see [38, Chapter IV, Theorem IV]) asserts that, for a given distribution $T \in \mathscr{S}'(\mathbb{R})$ and $\varphi \in \mathscr{S}(\mathbb{R})$,

$$\int_{\mathbb{R}} \langle T, \phi(\cdot, \omega) \rangle_{\mathscr{S}', \mathscr{S}} \, \varphi(\omega) \, \mathrm{d}\omega = \left\langle T, \int_{\mathbb{R}} \phi(\cdot, \omega)\varphi(\omega) \, \mathrm{d}\omega \right\rangle_{\mathscr{S}', \mathscr{S}}.$$

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When $T \in H^{-1}(\mathbb{R})$, the above linear form can be extended to functions in $H^1(\mathbb{R})$. Therefore, (106) can be rewritten as

$$\int_{\mathbb{R}} \operatorname{Re}\left(\widetilde{g}(\omega + \mathrm{i}\eta)\right)\varphi(\omega)\,\mathrm{d}\omega = \left\langle \operatorname{Im}\widehat{g}, \frac{1}{2\pi}\int_{\mathbb{R}} \frac{\cdot - \omega}{(\cdot - \omega)^2 + \eta^2}\varphi(\omega)\,\mathrm{d}\omega \right\rangle_{H^{-1}, H^1} \qquad (107)$$
$$+ \left\langle \operatorname{Re}\widehat{g}, \frac{1}{2\pi}\int_{\mathbb{R}} \frac{\eta}{(\cdot - \omega)^2 + \eta^2}\varphi(\omega)\,\mathrm{d}\omega \right\rangle_{H^{-1}, H^1}.$$

In view of the following strong convergences in $H^1(\mathbb{R})$,

$$\frac{1}{2\pi}\int_{\mathbb{R}} \frac{\xi - \omega}{(\xi - \omega)^2 + \eta^2}\,\varphi(\omega)\,\mathrm{d}\omega \xrightarrow[\eta \to 0]{} \frac{1}{2}(\mathfrak{H}\varphi)(\xi), \qquad \frac{1}{2\pi}\int_{\mathbb{R}} \frac{\eta}{(\xi - \omega)^2 + \eta^2}\,\varphi(\omega)\,\mathrm{d}\omega \xrightarrow[\eta \to 0]{} \frac{1}{2}\varphi(\xi),$$

the equality (107) leads, in the limit $\eta \to 0^+$, to

$$\langle \operatorname{Re}\widehat{g}, \varphi \rangle_{H^{-1}, H^1} = \frac{1}{2}\langle \operatorname{Im}\widehat{g}, \mathfrak{H}(\varphi) \rangle_{H^{-1}, H^1} + \frac{1}{2}\langle \operatorname{Re}\widehat{g}, \varphi \rangle_{H^{-1}, H^1}.$$

The first equality in the statement of item (iv) is finally obtained with the following lemma (recall that, according to Lemma 4, $H^s(\mathbb{R})$ is stable by the Hilbert transform). The second equality follows by applying $\mathfrak{H}$ to both sides and remembering that $\mathfrak{H}^2 = -\mathrm{Id}$.

Lemma 76. *Let $s \geqslant 0$. For any $T \in H^{-s}(\mathbb{R})$ and $\varphi \in H^s(\mathbb{R})$,*

$$\langle \mathfrak{H}(T), \varphi \rangle_{H^{-s}, H^s} = -\langle T, \mathfrak{H}(\varphi) \rangle_{H^{-s}, H^s}.$$

Proof. Consider first the case when $T, \varphi \in \mathscr{S}(\mathbb{R})$. Then, using Plancherel's formula, the duality product can be rewritten using a L^2-scalar product

$$\langle \mathfrak{H}T, \varphi \rangle_{\mathscr{S}', \mathscr{S}} = (\overline{\mathfrak{H}T}, \phi)_{L^2} = 2\pi\left(\overline{\mathcal{F}^{-1}(\mathfrak{H}T)}, \mathcal{F}^{-1}\varphi\right)_{L^2} = 2\pi\left(-\mathrm{i}\,\mathrm{sgn}(\cdot)\overline{\mathcal{F}^{-1}T}, \mathcal{F}^{-1}\varphi\right)_{L^2}$$
$$= 2\pi\left(\mathcal{F}^{-1}\overline{T}, \mathrm{i}\,\mathrm{sgn}(\cdot)\mathcal{F}^{-1}\varphi\right)_{L^2} = -\left(\overline{T}, \mathfrak{H}\varphi\right)_{L^2} = -\langle T, \mathfrak{H}\varphi \rangle_{\mathscr{S}', \mathscr{S}}.$$

The conclusion is obtained by a density argument. $\qquad\square$

6.3 Proof of Proposition 12

The proof presented in Section 6.2 can be followed *mutatis mutandis* upon introducing, for given elements $f, g \in \mathcal{H}$, the bounded causal function

$$a_{f,g}(\tau) = \langle f\,|T_{\mathrm{c}}(\tau)|\,g \rangle,$$

and noting that $\|a_{f,g}\|_{L^\infty} \leqslant \|T_{\mathrm{c}}\|_{L^\infty(\mathcal{B}(\mathcal{H}))}\|f\|\|g\|$.

The only additional technical point is the strong analyticity property, which is however easily obtained from the following bound: for $z = \omega + \mathrm{i}\eta \in \mathbb{U}$,

$$\left\|\frac{\mathrm{d}\widetilde{T}_{\mathrm{c}}(z)}{\mathrm{d}z}\right\|_{\mathcal{B}(\mathcal{H})} = \left\|\int_0^\infty T_{\mathrm{c}}(\tau)(\mathrm{i}\tau)\mathrm{e}^{-\eta\tau}\mathrm{e}^{\mathrm{i}\omega\tau}\,\mathrm{d}\tau\right\|_{\mathcal{B}(\mathcal{H})}$$
$$\leqslant \|T_{\mathrm{c}}\|_{L^\infty(\mathbb{R}_\tau, \mathcal{B}(\mathcal{H}))}\int_0^\infty \tau\mathrm{e}^{-\eta\tau}\,\mathrm{d}\tau = \frac{\|T_{\mathrm{c}}\|_{L^\infty(\mathbb{R}_\tau, \mathcal{B}(\mathcal{H}))}}{\eta^2} < +\infty.$$

6.4 Proof of Proposition 13

For $z \in \mathbb{U}$, we have

$$\widetilde{A}_{\mathrm{c}}(z) = \int_{\mathbb{R}} A_{\mathrm{c}}(\tau)\,\mathrm{e}^{\mathrm{i}z\tau}\,\mathrm{d}\tau = -\mathrm{i}\int_0^{+\infty} \mathrm{e}^{-\mathrm{i}\tau H}\mathrm{e}^{\mathrm{i}z\tau}\,\mathrm{d}\tau.$$

A simple computation shows that

$$\widetilde{A}_{\mathrm{c}}(\omega + \mathrm{i}\eta) = -\mathrm{i}\int_0^{+\infty}\int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}\tau(\omega+\mathrm{i}\eta-\lambda)}\,\mathrm{d}P_\lambda^H\,\mathrm{d}\tau = \int_{\mathbb{R}}\frac{1}{\omega+\mathrm{i}\eta-\lambda}\,\mathrm{d}P_\lambda^H = (\omega+\mathrm{i}\eta-H)^{-1}.$$

The series of equalities can be made rigorous by testing them against functions $f, g \in \mathcal{H}$, and using Fubini's theorem to justify the exchange in the order of integration.

The strong convergence of $\widetilde{A}_{\mathrm{c}}(\cdot + \mathrm{i}\eta)$ to $\widehat{A}_{\mathrm{c}}$ in $H^1(\mathbb{R}_\tau, \mathcal{B}(\mathcal{H}))$ is ensured by Proposition 12. The Fourier transform can therefore be deduced from this limiting procedure. We consider the limit of $\mathrm{Im}\,\widetilde{A}_{\mathrm{c}}(\cdot + \mathrm{i}\eta)$, the real part of $\widetilde{A}_{\mathrm{c}}(\cdot + \mathrm{i}\eta)$ being obtained from (14) and Definition 8.

Let $f \in \mathcal{H}$ and $\varphi \in \mathscr{S}(\mathbb{R}_\omega)$. Then, using Fubini's theorem,

$$\left\langle\left\langle f\,\Big|\,\mathrm{Im}\,\widetilde{A}_{\mathrm{c}}(\cdot+\mathrm{i}\eta)\Big|\,f\right\rangle, \varphi\right\rangle_{\mathscr{S}',\mathscr{S}} = -\int_{\mathbb{R}}\int_{\mathbb{R}}\frac{\eta}{(\omega-\lambda)^2+\eta^2}\,\varphi(\omega)\,\mu_f^H(\mathrm{d}\lambda)\,\mathrm{d}\omega = -\int_{\mathbb{R}}t_\eta(\lambda)\,\mu_f^H(\mathrm{d}\lambda), \tag{108}$$

where the measure μ_f^H is defined by $\mu_f^H(b) = \langle f\,|\,P_b^H\,|\,f\rangle$ for any $b \in \mathscr{B}(\mathbb{R})$, and

$$t_\eta(\lambda) = \int_{\mathbb{R}}\frac{\eta}{(\omega-\lambda)^2+\eta^2}\,\varphi(\omega)\,\mathrm{d}\omega = \int_{\mathbb{R}}\frac{1}{\xi^2+1}\,\varphi(\lambda+\eta\xi)\,\mathrm{d}\xi.$$

Note that

$$|t_\eta(\lambda)-\pi\varphi(\lambda)| \leqslant \int_{\mathbb{R}}\frac{1}{\xi^2+1}\,|\varphi(\lambda+\eta\xi)-\varphi(\lambda)|\,\mathrm{d}\xi \leqslant \sqrt{\eta}\|\varphi'\|_{L^2}\int_{\mathbb{R}}\frac{\sqrt{\xi}}{1+\xi^2}\,\mathrm{d}\xi,$$

where the last bound is obtained by rewriting $\varphi(\lambda+\eta\xi)-\varphi(\lambda)$ as the integral of its derivative and using a Cauchy-Schwarz inequality. This also shows that t_η is uniformly bounded as $\eta \to 0^+$. Since the measure μ_f^H is finite, (108) leads by dominated convergence to

$$\left\langle\left\langle f\,\Big|\,\mathrm{Im}\,\widetilde{A}_{\mathrm{c}}(\cdot+\mathrm{i}\eta)\Big|\,f\right\rangle, \varphi\right\rangle_{\mathscr{S}',\mathscr{S}} \xrightarrow[\eta\to 0]{} -\pi\int_{\mathbb{R}}\varphi(\lambda)\,\mu_f^H(\mathrm{d}\lambda),$$

which shows that $\mathrm{Im}\,\widehat{A}_{\mathrm{c}} = -\pi\,P^H$.

6.5 Proof of Lemma 14

Let us first assume that $\mathrm{Im}\,\widehat{T}_{\mathrm{c}} \geqslant 0$. The aim is to prove that $\mathrm{Re}\,\widehat{T}_{\mathrm{c}} \geqslant 0$ on $(-\infty, \omega_0]$. Consider to this end $\varphi \in \mathscr{S}(\mathbb{R})$ with $\mathrm{Supp}(\varphi) \subset (-\infty, \omega_0]$ and $\varphi \geqslant 0$. Then, for any $\omega \geqslant \omega_0$ and $\omega' \leqslant 0$, it holds $\varphi(\omega-\omega') = 0$, so that

$$\forall\omega \geqslant \omega_0, \qquad (\mathfrak{H}\varphi)(\omega) = \lim_{\varepsilon\to 0^+}\int_{\mathbb{R}\setminus[-\varepsilon,\varepsilon]}\frac{\varphi(\omega-\omega')}{\omega'}\,\mathrm{d}\omega' = \lim_{\varepsilon\to 0^+}\int_\varepsilon^{+\infty}\frac{\varphi(\omega-\omega')}{\omega'}\,\mathrm{d}\omega' \geqslant 0. \tag{109}$$

Let $f \in \mathcal{H}$. In view of (14) and Lemma 76,

$$\left\langle\left\langle f\,\Big|\,\mathrm{Re}\,\widehat{T}_{\mathrm{c}}\Big|\,f\right\rangle, \varphi\right\rangle_{H^{-1},H^1} = -\left\langle\left\langle f\,\Big|\,\mathfrak{H}\left(\mathrm{Im}\,\widehat{T}_{\mathrm{c}}\right)\Big|\,f\right\rangle, \varphi\right\rangle_{H^{-1},H^1} = -\left\langle\mathfrak{H}\left(\left\langle f\,\Big|\,\mathrm{Im}\,\widehat{T}_{\mathrm{c}}\Big|\,f\right\rangle\right), \varphi\right\rangle_{H^{-1},H^1}$$

$$= \left\langle\left\langle f\,\Big|\,\mathrm{Im}\,\widehat{T}_{\mathrm{c}}\Big|\,f\right\rangle, \mathfrak{H}\varphi\right\rangle_{H^{-1},H^1}.$$

The latter quantity is non-negative since $\mathrm{Im}\,\widehat{T}_{\mathrm{c}} \geqslant 0$ and $\mathfrak{H}\varphi \geqslant 0$ on $\mathrm{Supp}(\mathrm{Im}\,\widehat{T}_{\mathrm{c}}) \subset [\omega_0, +\infty)$ (by (109)).

Let us now assume that $\mathrm{Re}\,\widehat{T}_{\mathrm{c}} \geqslant 0$ on $(-\infty, \omega_0]$. The aim is to prove that $\mathrm{Im}\,\widehat{T}_{\mathrm{c}} \geqslant 0$ on the support of this distribution, which is included in $[\omega_0, +\infty)$. Consider therefore $\varphi \in \mathscr{S}(\mathbb{R})$ with $\mathrm{Supp}(\varphi) \subset [\omega_0, +\infty)$ and $\varphi \geqslant 0$. Note that

$$\forall\omega \leqslant \omega_0, \qquad (\mathfrak{H}\varphi)(\omega) = \lim_{\varepsilon\to 0^-}\int_{-\infty}^\varepsilon\frac{\varphi(\omega-\omega')}{\omega'}\,\mathrm{d}\omega' \leqslant 0,$$

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and, for any $f \in \mathcal{H}$,

$$\left\langle \left\langle f \left| \operatorname{Im} \widehat{T_{\mathrm{c}}} \right| f \right\rangle, \varphi \right\rangle_{H^{-1}, H^1} = -\left\langle \left\langle f \left| \operatorname{Re} \widehat{T_{\mathrm{c}}} \right| f \right\rangle, \mathfrak{H}\varphi \right\rangle_{H^{-1}, H^1} \geqslant 0.$$

This gives the desired conclusion.

6.6 Proof of Lemma 21

The fact that $B_1 \in \mathcal{B}(L^1(\mathbb{R}^2), L^2(\mathbb{R}^3))$ is a simple consequence of the following inequality: for $\varphi \in L^1(\mathbb{R}^3)$, it holds, for almost all $\mathbf{r} \in \mathbb{R}^3$,

$$|B_1\varphi(\mathbf{r})| = \left| \int_{\mathbb{R}^3} B_1(\mathbf{r}, \mathbf{r}')\varphi(\mathbf{r}')\mathrm{d}\mathbf{r}' \right| \leqslant \|B_1(\mathbf{r}, \cdot)\|_{L^\infty(\mathbb{R}^3)} \|\varphi\|_{L^1(\mathbb{R}^3)}.$$

This shows that $B_1\varphi \in L^2(\mathbb{R}^3)$ with

$$\|B_1\varphi\|_{L^2(\mathbb{R}^3)} \leqslant \left(\int_{\mathbb{R}^3} \|B_1(\mathbf{r}, \cdot)\|_{L^\infty(\mathbb{R}^3)}^2 \, \mathrm{d}\mathbf{r} \right)^{1/2} \|\varphi\|_{L^1(\mathbb{R}^3)}.$$

Now, for $f \in L^2(\mathbb{R}^3)$, it is easy to see that $B_1 f$ is an integral operator with kernel $B_1(\mathbf{r}, \mathbf{r}')f(\mathbf{r}')$. In addition,

$$\|B_1 f\|_{\mathfrak{S}_2(L^2(\mathbb{R}^3))}^2 = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} |B_1(\mathbf{r}, \mathbf{r}')f(\mathbf{r}')|^2 \, \mathrm{d}\mathbf{r} \, \mathrm{d}\mathbf{r}' \leqslant \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \|B_1(\mathbf{r}, \cdot)\|_{L^\infty(\mathbb{R}^3)}^2 |f(\mathbf{r}')|^2 \, \mathrm{d}\mathbf{r} \, \mathrm{d}\mathbf{r}'$$
$$= \left(\int_{\mathbb{R}^3} \|B_1(\mathbf{r}, \cdot)\|_{L^2(\mathbb{R}^3)}^2 \mathrm{d}\mathbf{r} \right) \|f\|_{L^2(\mathbb{R}^3)}^2.$$

This gives the claimed result.

6.7 Proof of Theorem 24

Fix $0 < \eta < \omega$ and $f, g \in \mathcal{H}$. We start from (24), which we rewrite as

$$\widetilde{C^+}(\nu + \mathrm{i}\omega) = \frac{\mathrm{i}}{2\pi} \int_{-\infty}^{+\infty} \widetilde{A^+}\big(\nu + \nu' - \omega' + \mathrm{i}(\omega - \eta)\big) \odot \widetilde{B^-}(\nu' - \omega' - \mathrm{i}\eta) \, \mathrm{d}\omega'. \qquad (110)$$

By Proposition 13 and Proposition 17,

$$\widetilde{A^+}(z) = A_1^*(z - A_2)^{-1}A_1, \qquad \widetilde{B^-}(z) = B_1^*(z + B_2)^{-1}B_1. \qquad (111)$$

The poles of $z \mapsto \widetilde{A^+}\big(\nu + \nu' + \mathrm{i}(\omega - \eta) - z\big)$ are located on the half-line $\mathrm{i}(\omega - \eta) + (-\infty, \nu + \nu' - a)$, while those of $z \mapsto \widetilde{B^-}(\nu' - \mathrm{i}\eta - z)$ are located on the half-line $-\mathrm{i}\eta + (b + \nu', +\infty)$. For any closed contour not enclosing any point of those two half-lines, the integral of $\widetilde{A^+}\big(\nu + \nu' + \mathrm{i}(\omega - \eta) - z\big) \odot \widetilde{B^-}(\nu' - \mathrm{i}\eta - z)$ on this contour vanishes. Let us choose the contour $\mathscr{C}_L$ plotted in Figure 6 and evaluate the contributions of the left-hand side of

$$\oint_{\mathscr{C}_L} \operatorname{Tr}_{\mathcal{H}} \left[\widetilde{A^+}\big(\nu + \nu' + \mathrm{i}(\omega - \eta) - z\big) g \widetilde{B^-}(\nu' - \mathrm{i}\eta - z)\overline{f} \right] \mathrm{d}z = 0, \qquad (112)$$

on the various segments. Recall that we choose $\nu < a + b$ and $\nu' \in (-b, a - \nu)$, so that $\nu + \nu' - a < 0 < \nu' + b$. Let us also emphasize that the operators appearing in the integrand do not have singularities.
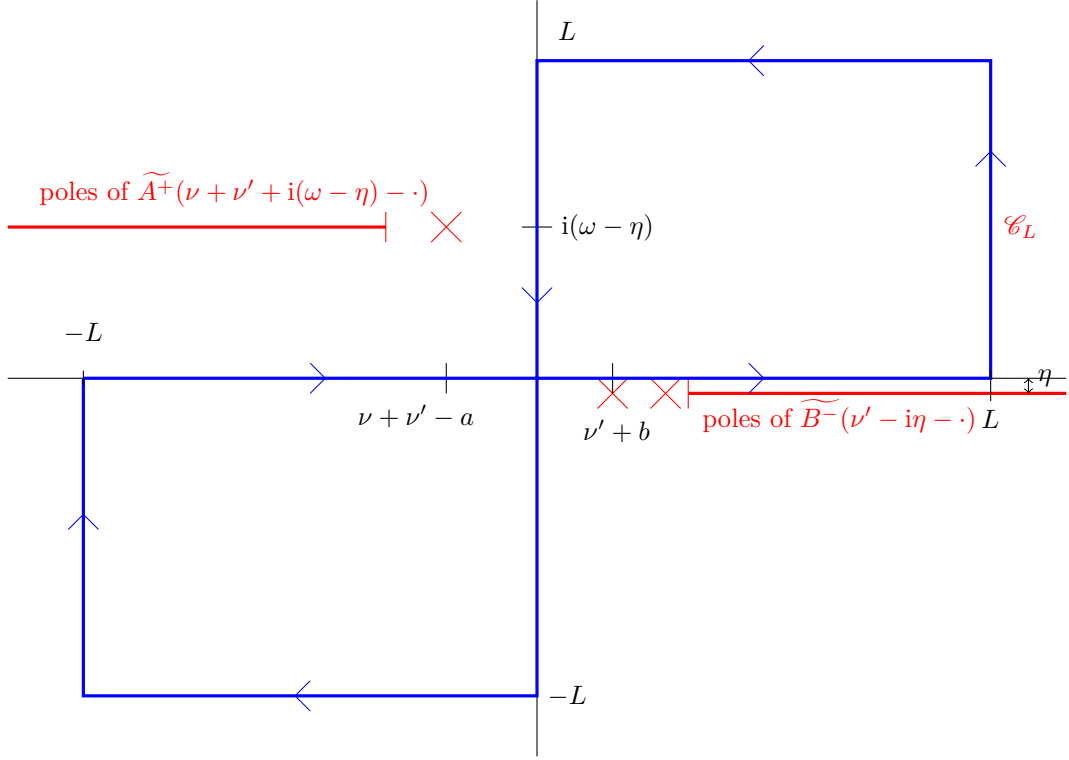
Figure 6: Contour $\mathscr{C}_L$ used to compute the integral (112), with $\eta > 0$ small compared to ω. Note that the condition $\nu + \nu' - a < 0 < \nu' + b$ ensures that the central vertical part of the contour does not intersect the poles of the functions in the integrand.

Let us first consider the part of the integral corresponding to the right side of the contour. Using (111), we obtain that for all $\omega' \in [0, L]$,

$$
\left| \int_0^L \mathrm{Tr}_{\mathcal{H}} \left[\widetilde{A^+}\big(\nu + \nu' - L + \mathrm{i}(\omega - \eta - \omega')\big) g \widetilde{B^-}\big(\nu' - L - \mathrm{i}(\omega' + \eta)\big) \overline{f} \right] \mathrm{d}\omega' \right|
$$

$$
\leqslant \int_0^L \left| \mathrm{Tr}_{\mathcal{H}} \left[A_1^* \frac{1}{\nu + \nu' - L + \mathrm{i}(\omega - \eta - \omega') - A_2} A_1 g B_1^* \frac{1}{\nu' - L - \mathrm{i}(\omega' + \eta) + B_2} B_1 \overline{f} \right] \right| \mathrm{d}\omega'
$$

$$
\leqslant \left\| B_1 \overline{f} \right\|_{\mathfrak{S}_2(\mathcal{H}, \mathcal{H}_b)} \left\| B_1 \overline{g} \right\|_{\mathfrak{S}_2(\mathcal{H}, \mathcal{H}_b)} \left\| A_1 \right\|_{\mathcal{B}(\mathcal{H}, \mathcal{H}_a)}^2
$$

$$
\times \int_0^L \left\| \frac{1}{\nu + \nu' - L + \mathrm{i}(\omega - \eta - \omega') - A_2} \right\|_{\mathcal{B}(\mathcal{H}_a)} \left\| \frac{1}{\nu' - L - \mathrm{i}(\omega' + \eta) + B_2} \right\|_{\mathcal{B}(\mathcal{H}_b)} \mathrm{d}\omega'
$$

$$
\leqslant C \|f\|_{\mathcal{H}} \|g\|_{\mathcal{H}} \frac{1}{L} \int_0^L \frac{\mathrm{d}\omega'}{\omega' + \eta} = C \|f\|_{\mathcal{H}} \|g\|_{\mathcal{H}} \frac{1}{L} \log\left(\frac{L + \eta}{\eta} \right),
$$

where we have used $A_2 - (\nu + \nu') + L \geqslant a - (\nu + \nu') + L \geqslant L$. Similar estimates can be stated for the upper, lower and left parts of the contour. For the upper part for instance, for which the

integration is performed from $z = L + \mathrm{i}L$ to $z = \mathrm{i}L$, we get

$$\left| \int_L^0 \mathrm{Tr}_{\mathcal{H}} \left[\widetilde{A^+}\big(\nu + \nu' - \omega' + \mathrm{i}(\omega - \eta - L)\big) g \widetilde{B^-}\big(\nu' - \omega' - \mathrm{i}(\eta + L)\big) \overline{f} \right] \mathrm{d}\omega' \right|$$

$$\leqslant C \|f\|_{\mathcal{H}} \|g\|_{\mathcal{H}} \int_0^L \left\| \frac{1}{\nu + \nu' - \omega' + \mathrm{i}(\omega - \eta - L) - A_2} \right\|_{\mathcal{B}(\mathcal{H}_a)} \left\| \frac{1}{\nu' - \omega' + \mathrm{i}(L + \eta) - B_2} \right\|_{\mathcal{B}(\mathcal{H}_b)} \mathrm{d}\omega'$$

$$\leqslant C \|f\|_{\mathcal{H}} \|g\|_{\mathcal{H}} \int_0^L \left(\frac{1}{L + \eta} \right) \frac{1}{\omega' + a - (\nu + \nu')} \mathrm{d}\omega'$$

$$= C \|f\|_{\mathcal{H}} \|g\|_{\mathcal{H}} \frac{\log\big(L + a - (\nu + \nu')\big) - \log\big(a - (\nu + \nu')\big)}{L + \eta},$$

where we recall that $a - (\nu + \nu') > 0$. We then take the limit $L \to +\infty$, so that the contributions to the integral which are not on the imaginary axis or on the real axis vanish. We deduce that

$$\int_{-\infty}^{\infty} \mathrm{Tr}_{\mathcal{H}} \left[\widetilde{A^+}\big(\nu + \nu' - \omega' + \mathrm{i}(\omega - \eta)\big) g \widetilde{B^-}(\nu' - \omega' - \mathrm{i}\eta) \overline{f} \right] \mathrm{d}\omega'$$

$$= \mathrm{i} \int_{-\infty}^{+\infty} \mathrm{Tr}_{\mathcal{H}} \left[\widetilde{A^+}\big(\nu + \nu' + \mathrm{i}(\omega - \eta + \omega')\big) g \widetilde{B^-}\big(\nu' + \mathrm{i}(\omega' - \eta)\big) \overline{f} \right] \mathrm{d}\omega'$$

$$= \mathrm{i} \int_{-\infty}^{+\infty} \mathrm{Tr}_{\mathcal{H}} \left[\widetilde{A^+}\big(\nu + \nu' + \mathrm{i}(\omega + \omega')\big) g \widetilde{B^-}(\nu' + \mathrm{i}\omega') \overline{f} \right] \mathrm{d}\omega'.$$

In view of (110), we finally obtain that

$$\widetilde{C^+}(\nu + \mathrm{i}\omega) = -\frac{1}{2\pi} \int_{-\infty}^{+\infty} \widetilde{A^+}\big(\nu + \nu' + \mathrm{i}(\omega + \omega')\big) \odot \widetilde{B^-}(\nu' + \mathrm{i}\omega') \, \mathrm{d}\omega'. \tag{113}$$

We next note that our choices for ν, ν' ensure that the expressions on both sides are analytic for all $\omega > 0$, and can be extended analytically to all $\omega \in \mathbb{R}$. Therefore, the above equality also holds true for $\omega \leqslant 0$.

In a similar fashion, we prove that, for all $\omega \in \mathbb{R}$,

$$\widetilde{C^-}(\nu + \mathrm{i}\omega) = -\frac{1}{2\pi} \int_{-\infty}^{+\infty} \widetilde{A^-}\big(\nu + \nu' + \mathrm{i}(\omega + \omega')\big) \odot \widetilde{B^+}(\nu' + \mathrm{i}\omega') \mathrm{d}\omega'.$$

This equality is established as for (113) by considering $\widetilde{C^-}(\nu - \mathrm{i}\omega)$ for $\omega > 0$ and evaluating the various parts of the left-hand side of

$$\oint_{\mathscr{C}_L} \mathrm{Tr}_{\mathcal{H}} \left[\widetilde{A^-}\big(\nu + \nu' - \mathrm{i}(\omega - \eta) - z\big) g \widetilde{B^+}(\nu' + \mathrm{i}\eta - z) \overline{f} \right] \mathrm{d}z = 0.$$

The poles of the integrand are on the half-lines $-\mathrm{i}(\omega - \eta) + (\nu + \nu' + a, +\infty)$ and $\mathrm{i}\eta + (-\infty, -b + \nu')$. The conditions $\nu > -(a + b)$ and $-a - \nu < \nu' < b$ ensure that $-b + \nu' < 0 < \nu + \nu' + a$, so that the integrand has no singularity on the imaginary axis.

Finally, since $A^+(\tau) \odot B^+(-\tau) = A^-(\tau) \odot B^-(-\tau) = 0$ for $\tau \neq 0$, we can concatenate $\widetilde{C^+}(\nu + \mathrm{i}\omega)$ and $\widetilde{C^-}(\nu + \mathrm{i}\omega)$, and obtain

$$\widetilde{C}(\nu + \mathrm{i}\omega) = -\frac{1}{2\pi} \int_{-\infty}^{+\infty} \widetilde{A}\big(\nu + \nu' + \mathrm{i}(\omega + \omega')\big) \odot \widetilde{B}(\nu' + \mathrm{i}\omega') \, \mathrm{d}\omega'.$$

6.8   Proof of Corollary 25

The proof is based on the representation (25) with the choice $\omega = 0$. Consider $\nu < a + b$. It holds

$$\widehat{C^+}(\nu) = \widetilde{C^+}(\nu) = -\frac{1}{2\pi} \int_{-\infty}^{+\infty} \widetilde{A^+}(\nu + \nu' + \mathrm{i}\omega') \odot \widetilde{B^-}(\nu' + \mathrm{i}\omega') \, \mathrm{d}\omega'$$

$$= -\frac{1}{2\pi} \int_{-\infty}^{+\infty} \left[A_1^* \frac{\nu + \nu' - A_2 - \mathrm{i}\omega'}{(\nu + \nu' - A_2)^2 + (\omega')^2} A_1 \right] \odot \left[B_1^* \frac{\nu' + B_2 - \mathrm{i}\omega'}{(\nu' + B_2)^2 + (\omega')^2} B_1 \right] \mathrm{d}\omega'.$$

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The odd terms in ω' cancel out by symmetry, so that

$$\widehat{C^+}(\nu) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \left[A_1^* \frac{A_2 - (\nu + \nu')}{(\nu + \nu' - A_2)^2 + (\omega')^2} A_1 \right] \odot \left[B_1^* \frac{\nu' + B_2}{(\nu' + B_2)^2 + (\omega')^2} B_1 \right] \mathrm{d}\omega'$$
$$+ \frac{1}{2\pi} \int_{-\infty}^{+\infty} \left[A_1^* \frac{\omega'}{(\nu + \nu' - A_2)^2 + (\omega')^2} A_1 \right] \odot \left[B_1^* \frac{\omega'}{(\nu' + B_2)^2 + (\omega')^2} B_1 \right] \mathrm{d}\omega'. \tag{114}$$

This shows that this operator is positive and self-adjoint in view of Lemmas 22 and 23. As a result, $\operatorname{Im} \widehat{C^+}(\nu) = 0$ for $\nu < a + b$. This proves the first assertion in (29). Also, we get from (114) that $\widehat{C^+}(\nu) = \operatorname{Re} \widehat{C^+} \geqslant 0$ for $\nu < a + b$. Together with Lemma 14, this shows the first assertion of (28). The results concerning $\operatorname{Im} \widehat{C^-}$ are proved in a similar way.

6.9 Proof of Proposition 26

The first assertion follows from the fact that the domain of H_N is $H^2(\mathbb{R}^{3N})$ and that $H_N \operatorname{Re}(\Psi_N^0) = E_N^0 \operatorname{Re}(\Psi_N^0)$ and $H_N \operatorname{Im}(\Psi_N^0) = E_N^0 \operatorname{Im}(\Psi_N^0)$.

The density ρ_N^0 is bounded since it decreases exponentially fast away from the nuclei and is continuous [13].

In order to prove (36), we rely on (31) and (34) in order to write (recall that Ψ_N^0 is real valued)

$$\left\langle \Psi_N^0 | a^\dagger(g) a(f) | \Psi_N^0 \right\rangle_{\mathcal{H}_N} = \left\langle a(g) \Psi_N^0 | a(f) \Psi_N^0 \right\rangle_{\mathcal{H}_N}$$
$$= N \int_{\mathbb{R}^{3(N-1)}} \left(\int_{\mathbb{R}^3} g(\mathbf{r}) \Psi_N^0(\mathbf{r}, \mathbf{r}_1, \dots, \mathbf{r}_{N-1}) \, \mathrm{d}\mathbf{r} \right) \left(\int_{\mathbb{R}^3} \overline{f(\mathbf{r}')} \Psi_N^0(\mathbf{r}', \mathbf{r}_1, \dots, \mathbf{r}_{N-1}) \, \mathrm{d}\mathbf{r}' \right) \mathrm{d}\mathbf{r}_1 \dots \mathrm{d}\mathbf{r}_{N-1}$$
$$= \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} g(\mathbf{r}) \gamma_N^0(\mathbf{r}, \mathbf{r}') \overline{f(\mathbf{r}')} \, \mathrm{d}\mathbf{r} \, \mathrm{d}\mathbf{r}' = \langle f | \gamma_N^0 | g \rangle.$$

To bound the kernel $|\gamma_N^0(\mathbf{r}, \mathbf{r}')|^2$, we write

$$|\gamma_N^0(\mathbf{r}, \mathbf{r}')|^2 = N^2 \left| \int_{\mathbb{R}^3} \dots \int_{\mathbb{R}^3} \Psi_N^0(\mathbf{r}, \mathbf{r}_2, \dots \mathbf{r}_N) \Psi_N^0(\mathbf{r}', \mathbf{r}_2, \dots \mathbf{r}_N) \mathrm{d}\mathbf{r}_2 \dots \mathrm{d}\mathbf{r}_N \right|^2$$
$$\leqslant N^2 \left(\int_{\mathbb{R}^3} \dots \int_{\mathbb{R}^3} |\Psi_N^0(\mathbf{r}, \mathbf{r}_2, \dots \mathbf{r}_N)|^2 \, \mathrm{d}\mathbf{r}_2 \dots \mathrm{d}\mathbf{r}_N \right) \left(\int_{\mathbb{R}^3} \dots \int_{\mathbb{R}^3} |\Psi_N^0(\mathbf{r}', \mathbf{r}_2, \dots \mathbf{r}_N)|^2 \, \mathrm{d}\mathbf{r}_2 \dots \mathrm{d}\mathbf{r}_N \right)$$
$$\leqslant \rho_N^0(\mathbf{r}) \rho_N^0(\mathbf{r}'),$$

where we used the Cauchy-Schwarz inequality.

Let us finally recall why $\rho_{N,2}^0$ defines a bounded integral operator. Note first that $\rho_{N,2}^0(\mathbf{r}, \mathbf{r}') \geqslant 0$. For $f, g \in \mathcal{H}_1$, the Cauchy-Schwarz inequality then leads to

$$\left| \langle f | \rho_{N,2}^0 | g \rangle \right| = \left| \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \overline{f(\mathbf{r})} \rho_{N,2}^0(\mathbf{r}, \mathbf{r}') g(\mathbf{r}') \, \mathrm{d}\mathbf{r} \, \mathrm{d}\mathbf{r}' \right|$$
$$\leqslant \left(\int_{\mathbb{R}^3} \int_{\mathbb{R}^3} |f(\mathbf{r})|^2 \rho_{N,2}^0(\mathbf{r}, \mathbf{r}') \, \mathrm{d}\mathbf{r} \, \mathrm{d}\mathbf{r}' \right)^{1/2} \left(\int_{\mathbb{R}^3} \int_{\mathbb{R}^3} |g(\mathbf{r}')|^2 \rho_{N,2}^0(\mathbf{r}, \mathbf{r}') \, \mathrm{d}\mathbf{r} \, \mathrm{d}\mathbf{r}' \right)^{1/2}$$
$$= \frac{(N-1)}{2} \left(\int_{\mathbb{R}^3} |f|^2 \, \rho_N^0 \right)^{1/2} \left(\int_{\mathbb{R}^3} |g|^2 \, \rho_N^0 \right)^{1/2}$$
$$\leqslant \frac{(N-1)}{2} \left\| \rho_N^0 \right\|_{L^\infty} \|f\|_{\mathcal{H}_1} \|g\|_{\mathcal{H}_1}.$$

This shows that $\rho_{N,2}^0$ defines a bounded operator on $\mathcal{H}_1$, with operator norm lower or equal to $(N-1) \left\| \rho_N^0 \right\|_{L^\infty} / 2$.

6.10 Proof of Theorem 36

Since

$$A_- f(\mathbf{r}_1, \ldots, \mathbf{r}_{N-1}) = \sqrt{N} \int_{\mathbb{R}^3} f(\mathbf{r}) \Psi_N^0(\mathbf{r}, \mathbf{r}_1, \ldots, \mathbf{r}_{N-1}) \, d\mathbf{r},$$

and introducing

$$\Delta_{N-1} = \sum_{i=1}^{N-1} \Delta_{\mathbf{r}_i},$$

it is easily seen that $(1 - \Delta_{N-1}) A_-$ is an integral operator with kernel $\left[(1 - \Delta_{N-1}) \Psi_N^0 \right] (\mathbf{r}_1, \ldots, \mathbf{r}_{N-1}; \mathbf{r})$. As $\Psi_N^0 \in H^2(\mathbb{R}^{3N})$, it follows that $(1 - \Delta_{N-1}) A_- \in \mathfrak{S}_2(\mathcal{H}_1, \mathcal{H}_{N-1})$. Therefore, any operator of the form $A_-^* B A_-$, where the operator B on $\mathcal{H}_{N-1}$ is such that $(1 - \Delta_{N-1})^{-1/2} B (1 - \Delta_{N-1})^{-1/2} \in \mathcal{B}(\mathcal{H}_1)$, is trace-class. In particular, the operator

$$\partial_\tau G_{\mathrm{h}}(\tau) \big|_{\tau=0^-} = -A_-^* (H_{N-1} - E_N^0) A_-,$$

is trace-class.

Let us now compute more explicitly the action of this operator. Let

$$h_1 := -\frac{1}{2} \Delta + v_{\mathrm{ext}}.$$

We use the definition (31) of $a(\overline{f})$, and obtain

$$\left(\sum_{i=1}^{N-1} h_1(\mathbf{r}_i) \right) \left[a(\overline{f}) \Psi_N^0 \right] (\mathbf{r}_1, \ldots, \mathbf{r}_{N-1}) = \sqrt{N} \int_{\mathbb{R}^3} f(\mathbf{r}_N) \left(\sum_{i=1}^{N-1} h_1(\mathbf{r}_i) \right) \Psi_N^0(\mathbf{r}_1, \ldots, \mathbf{r}_N) \, d\mathbf{r}_N$$

$$= \sqrt{N} \int_{\mathbb{R}^3} f(\mathbf{r}_N) \left(H_{0,N} \Psi_N^0 \right) (\mathbf{r}_1, \ldots, \mathbf{r}_N) \, d\mathbf{r}_N \qquad (115)$$

$$- \sqrt{N} \int_{\mathbb{R}^3} (h_1 f)(\mathbf{r}_N) \Psi_N^0(\mathbf{r}_1, \ldots, \mathbf{r}_N) \, d\mathbf{r}_N,$$

so that

$$(H_{N-1} A_- f) (\mathbf{r}_1, \ldots, \mathbf{r}_{N-1}) = E_N^0 (A_- f) (\mathbf{r}_1, \ldots, \mathbf{r}_{N-1}) - (A_- h_1 f) (\mathbf{r}_1, \ldots, \mathbf{r}_{N-1})$$

$$- \sqrt{N} \sum_{i=1}^{N-1} \int_{\mathbb{R}^3} f(\mathbf{r}) \frac{\Psi_N^0(\mathbf{r}, \mathbf{r}_1, \ldots, \mathbf{r}_{N-1})}{|\mathbf{r} - \mathbf{r}_i|} \, d\mathbf{r}.$$

Moreover, it is easily seen that, for any $\Phi_{N-1} \in \mathcal{H}_{N-1}$,

$$\left(A_-^* \Phi_{N-1} \right) (\mathbf{r}) = \sqrt{N} \int_{\mathbb{R}^{3(N-1)}} \Psi_N^0(\mathbf{r}, \mathbf{r}_1, \ldots, \mathbf{r}_{N-1}) \Phi_{N-1}(\mathbf{r}_1, \ldots, \mathbf{r}_{N-1}) \, d\mathbf{r}_1 \ldots d\mathbf{r}_{N-1}.$$

Therefore,

$$\left(A_-^* \left(H_{N-1} - E_N^0 \right) A_- f \right) (\mathbf{r}) = - \left(\gamma_N^0 h_1 f \right) (\mathbf{r}) - \int_{\mathbb{R}^3} K_N(\mathbf{r}, \mathbf{r}') f(\mathbf{r}') \, d\mathbf{r}',$$

with

$$K_N(\mathbf{r}, \mathbf{r}') = N \sum_{i=1}^{N-1} \int_{\mathbb{R}^{3(N-1)}} \frac{\Psi_N^0(\mathbf{r}, \mathbf{r}_1, \ldots, \mathbf{r}_{N-1}) \Psi_N^0(\mathbf{r}', \mathbf{r}_1, \ldots, \mathbf{r}_{N-1})}{|\mathbf{r}' - \mathbf{r}_i|} \, d\mathbf{r}_1 \ldots d\mathbf{r}_{N-1}.$$

Since we already know that the integral operator K_N on $\mathcal{H}_1$, with kernel $K_N(\mathbf{r}, \mathbf{r}')$ is trace-class, and that Ψ_N^0 is continuous and decays exponentially fast (see *e.g.* [13]), we have [40, Theorem A.2]

$$\mathrm{Tr}_{\mathcal{H}_1}(K_N) = \int_{\mathbb{R}^3} K_N(\mathbf{r}, \mathbf{r}) \, d\mathbf{r} = N(N-1) \int_{\mathbb{R}^{3(N-1)}} \frac{\left| \Psi_N^0(\mathbf{r}, \mathbf{r}_1, \ldots, \mathbf{r}_{N-1}) \right|^2}{|\mathbf{r} - \mathbf{r}_1|} \, d\mathbf{r}_1 \ldots d\mathbf{r}_{N-1}$$

$$= 2 \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\rho_{N,2}^0(\mathbf{r}, \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \, d\mathbf{r} \, d\mathbf{r}',$$

where we recall that $\rho_{N,2}^0$ is the two-body density matrix defined in (35).

Finally,

$$\mathrm{Tr}_{\mathcal{H}_1}\left(\partial_\tau G_{\mathrm{h}}(\tau)\big|_{\tau=0^-}\right) = -\mathrm{Tr}_{\mathcal{H}_1}\left(A_-^*(H_{N-1} - E_N^0)A_-\right)$$
$$= \mathrm{Tr}_{\mathcal{H}_1}\left(\gamma_N^0 h_1\right) + 2\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{\rho_{N,2}^0(\mathbf{r},\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\,\mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{r}',$$

which gives the claimed result in view of the following representation of the ground state energy:

$$E_N^0 = \langle\Psi_N^0|H_N|\Psi_N^0\rangle = \mathrm{Tr}_{\mathcal{H}_1}\left(h_1\gamma_N^0\right) + \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{\rho_{N,2}^0(\mathbf{r},\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\,\mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{r}'. \tag{116}$$

6.11 Proof of Lemma 42

Proposition 26 shows that $\rho_N^0 \in L^p(\mathbb{R}^3)$ for $1 \leqslant p \leqslant +\infty$. This implies that $\left(\sum_{i=1}^N v(\mathbf{r}_i)\right)\Psi_N^0$ belongs to $\mathcal{H}_N$ for $v \in \mathcal{C}'$ since, by Hölder's inequality, and the inequality $\left(\sum_{i=1}^N v(\mathbf{r}_i)\right)^2 \leqslant N\sum_{i=1}^N v(\mathbf{r}_i)^2$, it holds that

$$\int_{\mathbb{R}^{3N}}\left(\sum_{i=1}^N v(\mathbf{r}_i)\right)^2 |\Psi_N^0(\mathbf{r}_1,\ldots,\mathbf{r}_N)|^2\,\mathrm{d}\mathbf{r}_1\ldots\mathrm{d}\mathbf{r}_N \leqslant N\int_{\mathbb{R}^3}v^2\rho_N^0 \leqslant N\|v\|_{L^6}^2\|\rho_N^0\|_{L^{3/2}}$$
$$\leqslant NC_{\mathcal{C}'}\|v\|_{\mathcal{C}'}^2\|\rho_N^0\|_{L^{3/2}},$$

where we have used the embedding $\mathcal{C}' \hookrightarrow L^6(\mathbb{R}^3)$. Moreover, $\rho_N^0 \in L^{6/5}(\mathbb{R}^3) \hookrightarrow \mathcal{C}$, so that $\left|\langle v,\rho_N^0\rangle_{\mathcal{C}',\mathcal{C}}\right| \leqslant \|v\|_{\mathcal{C}'}\|\rho_N^0\|_{\mathcal{C}}$. We therefore deduce that B is a bounded operator from $\mathcal{C}'$ to $\mathcal{H}_N$, whose norm satisfies

$$\|B\|_{\mathcal{B}(\mathcal{C}',\mathcal{H}_N)} \leqslant \sqrt{NC_{\mathcal{C}'}\|\rho_N^0\|_{L^{3/2}}} + \|\rho_N^0\|_{\mathcal{C}}.$$

We finally have, for $v \in \mathcal{C}'$,

$$\left\langle \Psi_N^0\left|\sum_{i=1}^N v(\mathbf{r}_i)\right|\Psi_N^0\right\rangle_{\mathcal{H}_N} = \int_{\mathbb{R}^3}v(\mathbf{r})\rho_N^0(\mathbf{r})\,\mathrm{d}\mathbf{r} = \langle v,\rho_N^0\rangle_{\mathcal{C}',\mathcal{C}}$$

from which we deduce that $\langle\Psi_N^0|Bv\rangle_{\mathcal{H}_N} = 0$. Since v was arbitrary, we conclude that $B^*\Psi_N^0 = 0$.

6.12 Proof of Theorem 46

Consider $f,g \in C_c^\infty(\mathbb{R}^3,\mathbb{C})$ (that is C^∞ with compact supports). Using the fact that $(H_N - E_N^0)|\Psi_N^0\rangle = 0$, we obtain

$$\langle\overline{f},v_c^{-1}B^*(H_N - E_N^0)Bg\rangle_{\mathcal{C}',\mathcal{C}} = \langle f\left|B^*(H_N - E_N^0)B\right|g\rangle_{\mathcal{C}'} = \langle Bf\left|H_N - E_N^0\right|Bg\rangle_{\mathcal{H}_N}$$
$$= \left\langle\Psi_N^0\left|\left(\sum_{j=1}^N\overline{f(\mathbf{r}_j)}\right)(H_N - E_N^0)\left(\sum_{i=1}^N g(\mathbf{r}_i)\right)\right|\Psi_N^0\right\rangle_{\mathcal{H}_N}.$$

We next observe that

$$(H_N - E_N^0)\left(\sum_{i=1}^N g(\mathbf{r}_i)\Psi_N^0(\mathbf{r}_1,\ldots,\mathbf{r}_N)\right) =$$
$$= \left(-\frac{1}{2}\sum_{i=1}^N \Delta g(\mathbf{r}_i)\right)\Psi_N^0(\mathbf{r}_1,\ldots,\mathbf{r}_N) - \sum_{i=1}^N \nabla g(\mathbf{r}_i)\cdot\nabla_{\mathbf{r}_i}\Psi_N^0(\mathbf{r}_1,\ldots,\mathbf{r}_N),$$

so that, using the fact that Ψ_N^0 is real-valued (see Proposition 26),

$$\langle f \,|\, B^*(H_N - E_N^0)B \,|\, g\rangle_{\mathcal{C}'} = \sum_{i,j=1}^N \int_{\mathbb{R}^{3N}} \overline{f(\mathbf{r}_j)}\left(-\frac{1}{2}\Delta g(\mathbf{r}_i)\right)|\Psi_N^0(\mathbf{r}_1,\dots \mathbf{r}_N)|^2\,\mathrm{d}\mathbf{r}_1\dots\mathrm{d}\mathbf{r}_N$$

$$-\sum_{i,j=1}^N \int_{\mathbb{R}^{3N}} \overline{f(\mathbf{r}_j)}\Psi_N^0(\mathbf{r}_1,\dots,\mathbf{r}_N)\nabla g(\mathbf{r}_i)\cdot\nabla_{\mathbf{r}_i}\Psi_N^0(\mathbf{r}_1,\dots,\mathbf{r}_N)\,\mathrm{d}\mathbf{r}_1\dots\mathrm{d}\mathbf{r}_N$$

$$= \frac{1}{2}\sum_{i=1}^N \int_{\mathbb{R}^{3N}} \overline{\nabla f(\mathbf{r}_j)}\cdot\nabla g(\mathbf{r}_i)|\Psi_N^0(\mathbf{r}_1,\dots \mathbf{r}_N)|^2\mathrm{d}\mathbf{r}_1\dots\mathrm{d}\mathbf{r}_N$$

$$+ \frac{1}{2}\sum_{i,j=1}^N \int_{\mathbb{R}^{3N}} \overline{f(\mathbf{r}_j)}\nabla g(\mathbf{r}_i)\cdot\nabla_{\mathbf{r}_i}\left(\left|\Psi_N^0(\mathbf{r}_1,\dots,\mathbf{r}_N)\right|^2\right)\mathrm{d}\mathbf{r}_1\dots\mathrm{d}\mathbf{r}_N$$

$$- \sum_{i,j=1}^N \int_{\mathbb{R}^{3N}} \overline{f(\mathbf{r}_j)}\Psi_N^0(\mathbf{r}_1,\dots,\mathbf{r}_N)\nabla g(\mathbf{r}_i)\cdot\nabla_{\mathbf{r}_i}\Psi_N^0(\mathbf{r}_1,\dots,\mathbf{r}_N)\mathrm{d}\mathbf{r}_1\dots\mathrm{d}\mathbf{r}_N$$

$$= \frac{1}{2}\int_{\mathbb{R}^3} \overline{\nabla f(\mathbf{r})}\cdot\nabla g(\mathbf{r})\rho_N^0(\mathbf{r})\mathrm{d}\mathbf{r}.$$

We deduce that $2v_c^{-1}B^*(H_N - E_N^0)B = 2v_c^{-1}B^*(H_N^\sharp - E_N^0)B = -\mathrm{div}\left(\rho_N^0\nabla\cdot\right)$ as operators on the core $C_c^\infty(\mathbb{R}^3,\mathbb{C})$. We next observe that $\mathrm{div}\left(\rho_N^0\nabla\cdot\right)$ can be extended as a bounded operator from $\mathcal{C}'$ to $\mathcal{C}$. Indeed, for $f,g \in C_c^\infty(\mathbb{R}^3,\mathbb{C})$,

$$\left|\langle g, \mathrm{div}\left(\rho_N^0\nabla f\right)\rangle_{\mathcal{C}',\mathcal{C}}\right| \leqslant \|\rho_N^0\|_{L^\infty}\|\nabla f\|_{L^2}\|\nabla g\|_{L^2} = 4\pi\|\rho_N^0\|_{L^\infty}\|f\|_{\mathcal{C}'}\|g\|_{\mathcal{C}'},$$

which shows that

$$\left\|\mathrm{div}\left(\rho_N^0\nabla\cdot\right)\right\|_{\mathcal{B}(\mathcal{C}',\mathcal{C})} \leqslant 4\pi\left\|\rho_N^0\right\|_{L^\infty}.$$

Therefore, $2v_c^{-1}B^*(H_N^\sharp - E_N^0)B = -\mathrm{div}\left(\rho_N^0\nabla\cdot\right)$ as bounded operators from $\mathcal{C}'$ to $\mathcal{C}$.

For the second part of the proof, we first note that it is sufficient to check the convergence in the case when $f = g \in C_c^\infty(\mathbb{R}^3,\mathbb{R})$. It holds:

$$\left\langle \overline{f}, v_c^{-1}B^*\frac{H_N^\sharp - E_N^0}{(H_N^\sharp - E_N^0)^2 + \omega^2}\omega^2 Bf\right\rangle_{\mathcal{C}',\mathcal{C}} - \langle \overline{f}, v_c^{-1}B^*(H_N^\sharp - E_N^0)Bf\rangle_{\mathcal{C}',\mathcal{C}}$$

$$= -\left\langle \overline{f}, v_c^{-1}B^*\left(\frac{(H_N^\sharp - E_N^0)^3}{(H_N^\sharp - E_N^0)^2 + \omega^2}\right)Bf\right\rangle_{\mathcal{C}',\mathcal{C}} = -\int_0^{+\infty}\left(\frac{\lambda^3}{\lambda^2 + \omega^2}\right)\mathrm{d}\left\|P_\lambda^{H_N^\sharp - E_N^0}(Bf)\right\|_{\mathcal{H}_N}^2,$$

where we used the spectral decomposition of $H_N^\sharp - E_N^0$ in the last equality. The integrand of the last integral converges pointwise to 0 when $|\omega|\to+\infty$. It is also non-negative and uniformly bounded by $\lambda\mathbb{1}_{[0,+\infty)}(\lambda)$, which is integrable since

$$\int_0^{+\infty}\lambda\,\mathrm{d}\left\|P_\lambda^{(H_N^\sharp - E_N^0)}(Bf)\right\|_{\mathcal{H}_N}^2 = \left\langle \overline{f}, v_c^{-1}B^*\left(H_N^\sharp - E_N^0\right)Bf\right\rangle_{\mathcal{C}',\mathcal{C}} = \frac{1}{2}\int_{\mathbb{R}^3}\rho_N^0|\nabla f|^2 < \infty.$$

The weak convergence therefore follows from the dominated convergence theorem.

To prove the strong convergence, we use the following rewriting for $g \in \mathcal{C}'$:

$$v_c^{-1}B^*\left(\frac{(H_N^\sharp - E_N^0)^3}{(H_N^\sharp - E_N^0)^2 + \omega^2}\right)Bg = v_c^{-1}B^*A_\omega Mg,$$

where

$$A_\omega = \frac{(H_N^\sharp - E_N^0)^2}{(H_N^\sharp - E_N^0)^2 + \omega^2}$$

strongly converge to 0 on $\mathcal{H}_N$, and

$$Mg := (H_N^\sharp - E_N^0)Bg = \sum_{i=1}^N \left(-\frac{1}{2}\Delta g(\mathbf{r}_i)\Psi_N^0 - \nabla g(\mathbf{r}_i)\cdot\nabla_{\mathbf{r}_i}\Psi_N^0 \right).$$

When $g \in \mathcal{C}'$ is such that $\Delta g \in L^2$, it holds that $Mg \in \mathcal{H}_N$ (by a proof similar to the one in Section 6.11), which allows us to conclude.

6.13 Proof of Proposition 48

We first prove (68) and (69). We start from an expression similar to the one provided by Lemma 38:

$$\widetilde{G_0}(z) := A_{0,+}\left(z - (H_{0,N+1} - E_{0,N}^0)\right)^{-1}A_{0,+}^* + A_{0,-}^*\left(z + H_{0,N-1} - E_{0,N}^0\right)^{-1}A_{0,-}.$$

Then, we notice that, for $f \in \mathcal{H}_1$, it holds

$$\sum_{i=1}^{N+1} h_1(\mathbf{r}_i)\left(A_{0,+}^* f\right) = \sum_{i=1}^{N+1} h_1(\mathbf{r}_i)\left(a^\dagger(f)|\Phi_N^0\rangle\right) = a^\dagger(h_1 f)\,|\Phi_N^0\rangle + a^\dagger(f)\left|\left(\sum_{i=1}^N h_1(\mathbf{r}_i)\right)\Phi_N^0\right\rangle, \quad (117)$$

or, equivalently,

$$H_{0,N+1}A_{0,+}^*(f) = A_{0,+}^*(h_1 f) + E_{0,N}^0 A_{0,+}^*(f);$$

so that

$$\left(z - (H_{0,N+1} - E_{0,N}^0)\right)A_{0,+}^* = A_{0,+}^*(z - h_1). \quad (118)$$

Hence, the particle part of (68) is a consequence of the equality $A_{0,+}A_{0,+}^* = \mathbb{1}_\mathcal{H} - \gamma_{0,N}^0$ (similarly to (39)). To handle the hole part, we use computations similar to (115), and find

$$H_{0,N-1}A_{0,-}(f) = E_{0,N}^0 A_{0,-}(f) - A_{0,-}(h_1 f).$$

We deduce that

$$(z + H_{0,N-1} - E_{0,N}^0)A_{0,-} = A_{0,-}(z - h_1), \quad (119)$$

and we conclude using the fact that $A_{0,-}^* A_{0,-} = \gamma_{0,N}^0$. Combining (118) and (119) leads to $\widetilde{G_0}(z)(z - h_1) = A_{0,-}^* A_{0,-} + A_{0,+}A_{0,+}^* = \mathbb{1}_{\mathcal{H}_1}$. Upon replacing z by $\overline{z}$ and passing to adjoints, it also follows $(z - h_1)\widetilde{G_0}(z) = \mathbb{1}_{\mathcal{H}_1}$. This shows that $\widetilde{G_0}(z) = (z - h_1)^{-1}$.

To prove the first assertion of Proposition 48, we notice that the operator-valued functions $\tau \mapsto -\mathrm{i}\Theta(\tau)\left(\mathbb{1}_{\mathcal{H}_1} - \gamma_{0,N}^0\right)\mathrm{e}^{-\mathrm{i}\tau h_1}$ and $\tau \mapsto G_{0,\mathrm{p}}(\tau)$ have the same Laplace transforms (see Proposition 13). We conclude that the two operators coincide since the Laplace transform is one-to-one. The proof for $G_{0,\mathrm{h}}$ is similar.

6.14 Proof of Proposition 50

Let $z \in \mathbb{C}\setminus\mathbb{R}$. Let us first prove that $\widetilde{G}(z)$ is a one-to-one operator. Let $f \in \mathcal{H}_1$ be such that $\widetilde{G}(z)f = 0$. From

$$\mathrm{Im}\left(\left\langle f\left|\widetilde{G}(z)\right|f\right\rangle\right) = \mathrm{Im}\left(\left\langle A_+^* f\left|\left(z - (H_{N+1} - E_N^0)\right)^{-1}\right|A_+^* f\right\rangle_{\mathcal{H}_{N+1}}\right. \quad (120)$$

$$\left. + \left\langle A_- f\left|\left(z - (E_N^0 - H_{N-1})\right)^{-1}\right|A_- f\right\rangle_{\mathcal{H}_{N-1}}\right)$$

$$= -\mathrm{Im}(z)\int_\mathbb{R}\left((\mathrm{Re}(z) + E_N^0 - \lambda)^2 + \mathrm{Im}(z)^2\right)^{-1}\mathrm{d}\left\|P_\lambda^{H_{N+1}}\left(A_+^* f\right)\right\|_{\mathcal{H}_{N+1}}^2$$

$$- \mathrm{Im}(z)\int_\mathbb{R}\left((\mathrm{Re}(z) - E_N^0 + \lambda)^2 + \mathrm{Im}(z)^2\right)^{-1}\mathrm{d}\left\|P_\lambda^{H_{N-1}}\left(A_- f\right)\right\|_{\mathcal{H}_{N-1}}^2,$$

$$(121)$$

we deduce that both terms in the right-hand side must vanish. In particular, since $\text{Im}(z) \neq 0$, it must hold $A_+^* f = A_- f = 0$. In view of the identity $A_-^* A_- + A_+ A_+^* = \mathbb{1}_{\mathcal{H}_1}$, this implies $f = 0$. Hence, $\widetilde{G}(z)$ is one-to-one.

As a consequence, $\widetilde{G}(z)$ is an invertible operator from $\mathcal{H}_1$ to its image $\widetilde{D}(z)$. Since $\left(\widetilde{G}(z)\right)^* = \widetilde{G}(\overline{z})$ is also one-to-one, $\widetilde{D}(z)$ is dense in $\mathcal{H}_1$.

Let us finally prove that $\widetilde{D}(z) \subset H^2(\mathbb{R}^3)$. We use to this end the equality (51). Let us consider the first term in this equality. A simple computation shows that, for any $\Phi_{N+1} \in \mathcal{H}_{N+1}$,

$$(A_+ \Phi_{N+1})(\mathbf{r}) = \sqrt{N+1} \int_{\mathbb{R}^{3N}} \Phi_{N+1}(\mathbf{r}, \mathbf{r}_1, \ldots, \mathbf{r}_N) \Psi_N^0(\mathbf{r}_1, \ldots, \mathbf{r}_N) \, d\mathbf{r}_1 \ldots d\mathbf{r}_N,$$

so that A_+ is a bounded operator from $H^2(\mathbb{R}^{3N}) \cap \mathcal{H}_N$ to $H^2(\mathbb{R}^3)$. Since A_+^* is a bounded operator from $\mathcal{H}_1$ to $\mathcal{H}_{N+1}$ and $(z - H_{N+1} + E_N^0)^{-1}$ is a bounded operator from $\mathcal{H}_{N+1}$ to $H^2(\mathbb{R}^{3N}) \cap \mathcal{H}_N$, we deduce that $A_+(z - H_{N+1} + E_N^0)^{-1} A_+^*$ is a bounded operator from $\mathcal{H}_1$ to $H^2(\mathbb{R}^3)$. Similarly, for any $\Phi_{N-1} \in \mathcal{H}_{N-1}$,

$$\left(A_-^* \Phi_{N-1}\right)(\mathbf{r}) = \sqrt{N} \int_{\mathbb{R}^{3(N-1)}} \Phi_{N-1}(\mathbf{r}_2, \ldots, \mathbf{r}_N) \Psi_N^0(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N) \, d\mathbf{r}_2 \ldots d\mathbf{r}_N,$$

so that A_-^* is a bounded operator from $\mathcal{H}_{N-1}$ to $H^2(\mathbb{R}^3)$. This allows us to prove that $A_-^*(z + H_{N-1} - E_N^0)^{-1} A_-$ is a bounded operator from $\mathcal{H}_1$ to $H^2(\mathbb{R}^3)$. Finally, $\widetilde{G}(z)$ is a bounded operator from $\mathcal{H}_1$ to $H^2(\mathbb{R}^3)$, which proves that $\widetilde{D}(z) \subset H^2(\mathbb{R}^3)$.

6.15   Proof of Lemma 56

Let us first prove that $\left(P_{\mathrm{sym}}^{0,+}(\tau)\right)_{\tau \in \mathbb{R}}$ defines a bounded causal operator. The proof is similar for $\left(P_{\mathrm{sym}}^{0,-}(\tau)\right)_{\tau \in \mathbb{R}}$. We rely on the following result.

Lemma 77. *For all $h \in L^6(\mathbb{R}^3)$, the operator $\gamma_{0,N}^0 h$ is a Hilbert-Schmidt operator on $\mathcal{H}_1$, and there exists $K \in \mathbb{R}^+$ such that*

$$\forall h \in L^6(\mathbb{R}^3), \quad \left\|\gamma_{0,N}^0 h\right\|_{\mathfrak{S}_2(\mathcal{H}_1)} \leqslant K \|h\|_{L^6}.$$

Proof of Lemma 77. Since $\gamma_{0,N}^0$ is a projector, for $h \in L^6(\mathbb{R}^3)$, the operator

$$\overline{h} \gamma_{0,N}^0 \gamma_{0,N}^0 h = \overline{h}(1-\Delta)^{-1/2}(1-\Delta)^{1/2} \gamma_{0,N}^0 (1-\Delta)^{1/2}(1-\Delta)^{-1/2} h$$

is the composition of $(1-\Delta)^{1/2} \gamma_{0,N}^0 (1-\Delta)^{1/2} \in \mathfrak{S}_1(\mathcal{H}_1)$ with the bounded operators $(1-\Delta)^{-1/2} h$ and $\overline{h}(1-\Delta)^{-1/2}$. In fact $(1-\Delta)^{-1/2} h \in \mathfrak{S}_6(\mathcal{H}_1)$ with

$$\left\|(1-\Delta)^{-1/2} h\right\|_{\mathfrak{S}_6(\mathcal{H}_1)} \leqslant K \|h\|_{L^6}$$

by the Kato-Seiler-Simon inequality [39, 40]. Therefore, $\gamma_{0,N}^0 h \in \mathfrak{S}_2(\mathcal{H}_1)$ with

$$\left\|\gamma_{0,N}^0 h\right\|_{\mathfrak{S}_2(\mathcal{H}_1)} \leqslant K \|h\|_{L^6},$$

which concludes the proof. $\qquad\square$

We now proceed to the proof of Lemma 56. We first note that, for $f, g \in C_c^\infty(\mathbb{R}^3, \mathbb{C})$, it holds

$$\langle f | v_c^{1/2} g \rangle_{\mathcal{H}_1} = \langle v_c^{-1/2} f | g \rangle_{\mathcal{C}} = \langle v_c^{1/2} \overline{f}, g \rangle_{\mathcal{C}', \mathcal{C}}. \tag{122}$$

In particular, for $\tau \in \mathbb{R}_\tau^+$, and for $f, g \in \mathcal{H}_1$, we get

$$\langle f | P_{\mathrm{sym}}^{0,+}(\tau) g \rangle_{\mathcal{H}_1} = \left\langle f \Big| v_c^{1/2} P^{0,+}(\tau) v_c^{1/2} g \right\rangle_{\mathcal{H}_1} = -\mathrm{i}\Theta(\tau) \left\langle v_c^{1/2} \overline{f}, G_{0,\mathrm{p}}(\tau) \odot G_{0,\mathrm{h}}(-\tau) v_c^{1/2} g \right\rangle_{\mathcal{C}', \mathcal{C}}$$

$$= -\mathrm{i}\Theta(\tau) \mathrm{Tr}_{\mathcal{H}_1} \left[G_{0,\mathrm{p}}(\tau) \left(v_c^{1/2} g\right) G_{0,\mathrm{h}}(-\tau) \left(v_c^{1/2} \overline{f}\right) \right].$$

Let us prove that $G_{0,\mathrm{p}}(\tau)\left(v_c^{1/2}g\right)G_{0,\mathrm{h}}(-\tau)\left(v_c^{1/2}\overline{f}\right)$ is indeed a trace-class operator. Replacing $G_{0,\mathrm{p}}$ and $G_{0,\mathrm{h}}$ by their expressions found in Proposition 48, and owing to the fact that $\gamma_{0,N}^0$ is a projector commuting with h_1, we obtain

$$
\begin{aligned}
\left|\langle f|P_{\mathrm{sym}}^{0,+}(\tau)|g\rangle\right| &= \left|\mathrm{Tr}_{\mathcal{H}_1}\left((\mathbb{1}_{\mathcal{H}_1}-\gamma_{0,N}^0)\mathrm{e}^{-\mathrm{i}\tau h_1}\left(v_c^{1/2}g\right)\gamma_{0,N}^0\mathrm{e}^{\mathrm{i}\tau h_1}\gamma_{0,N}^0\gamma_{0,N}^0\left(v_c^{1/2}\overline{f}\right)\right)\right| \\
&\leqslant \left\|(\mathbb{1}_{\mathcal{H}_1}-\gamma_{0,N}^0)\mathrm{e}^{-\mathrm{i}\tau h_1}\right\|_{\mathcal{B}(\mathcal{H}_1)}\left\|\mathrm{e}^{\mathrm{i}\tau h_1}\right\|_{\mathcal{B}(\mathcal{H}_1)} \\
&\quad \times \left\|\gamma_{0,N}\left(v_c^{1/2}\overline{f}\right)\right\|_{\mathcal{B}(\mathcal{H}_1)}\left\|\gamma_{0,N}\left(v_c^{1/2}g\right)\right\|_{\mathcal{B}(\mathcal{H}_1)}\left\|\gamma_{0,N}^0\right\|_{\mathfrak{S}_1(\mathcal{H}_1)}.
\end{aligned}
$$

According to Lemma 41, $v_c^{1/2}\overline{f}\in\mathcal{C}'\hookrightarrow L^6(\mathbb{R}^3)$. Therefore, $\gamma_{0,N}^0\left(v_c^{1/2}f\right)\in\mathfrak{S}_2(\mathcal{H}_1)$ by Lemma 77, hence is bounded, with

$$
\left\|\gamma_{0,N}^0\left(v_c^{1/2}f\right)\right\|_{\mathcal{B}(\mathcal{H}_1)}\leqslant\left\|\gamma_{0,N}^0\left(v_c^{1/2}f\right)\right\|_{\mathfrak{S}_2(\mathcal{H}_1)}\leqslant C\left\|v_c^{1/2}\overline{f}\right\|_{L^6}\leqslant\widetilde{C}\|f\|_{\mathcal{H}_1}.
$$

Similarly, $\left\|\left(v_c^{1/2}g\right)\gamma_{0,N}^0\right\|_{\mathcal{B}(\mathcal{H}_1)}\leqslant\widetilde{C}\|g\|_{\mathcal{H}_1}$. Altogether, we found a constant $C\in\mathbb{R}^+$ independent of τ such that

$$
\forall f,g\in\mathcal{H}_1,\quad\left|\langle f|P_{\mathrm{sym}}^{0,+}(\tau)|g\rangle\right|\leqslant C\|f\|_{\mathcal{H}_1}\|g\|_{\mathcal{H}_1},
$$

which proves that $\left(P_{\mathrm{sym}}^{0,+}(\tau)\right)_{\tau\in\mathbb{R}}$ is a bounded causal operator on $\mathcal{H}_1$.

Let us now prove that ϕ_k is a bounded operator from $\mathcal{H}_1$ to $\mathcal{C}$. Recall that ϕ_k is real-valued and $\phi_k\in H^2(\mathbb{R}^3)\subset L^2(\mathbb{R}^3,\mathbb{R})\cap L^\infty(\mathbb{R}^3,\mathbb{R})$ for $1\leqslant k\leqslant N$. For $f\in\mathcal{H}_1$, we obtain

$$
\|\phi_k f\|_{\mathcal{C}}\leqslant C\|\phi_k f\|_{L^{6/5}}\leqslant C\|\phi_k\|_{L^3}\|f\|_{\mathcal{H}_1},
$$

where C is a constant independent of f. The proof that ϕ_k is also a bounded operator from $\mathcal{C}'$ to $\mathcal{H}_1$ is similar, noticing that $\mathcal{C}'\hookrightarrow L^6(\mathbb{R}^3)$. We now use (80), and find that, for $f,g\in\mathcal{H}_1$ and for $\tau\in\mathbb{R}_\tau^+$,

$$
\begin{aligned}
\langle f|P_{\mathrm{sym}}^{0,+}(\tau)|g\rangle &= -\mathrm{i}\sum_{k=1}^N\mathrm{Tr}_{\mathcal{H}_1}\left((\mathbb{1}_{\mathcal{H}_1}-\gamma_{0,N}^0)\mathrm{e}^{-\mathrm{i}\tau h_1}\left(v_c^{1/2}g\right)|\phi_k\rangle\mathrm{e}^{\mathrm{i}\tau\varepsilon_k}\langle\phi_k|\left(v_c^{1/2}\overline{f}\right)\right) \\
&= -\mathrm{i}\sum_{k=1}^N\mathrm{Tr}_{\mathcal{H}_1}\left((\mathbb{1}_{\mathcal{H}_1}-\gamma_{0,N}^0)\mathrm{e}^{-\mathrm{i}\tau(h_1-\varepsilon_k)}\left|\left(v_c^{1/2}g\right)\phi_k\right\rangle\left\langle\left(v_c^{1/2}f\right)\phi_k\right|\right) \\
&= -\mathrm{i}\sum_{k=1}^N\left\langle\left(v_c^{1/2}f\right)\phi_k\right|(\mathbb{1}_{\mathcal{H}_1}-\gamma_{0,N}^0)\mathrm{e}^{-\mathrm{i}\tau(h_1-\varepsilon_k)}(\mathbb{1}_{\mathcal{H}_1}-\gamma_{0,N}^0)\left|\left(v_c^{1/2}g\right)\phi_k\right\rangle, \quad(123)
\end{aligned}
$$

which gives (81).

We finally prove that $P_{\mathrm{sym}}^{0,-}(\tau)=P_{\mathrm{sym}}^{0,+}(-\tau)$. Performing similar calculation as for $P_{\mathrm{sym}}^{0,+}$, we find that, for $f,g\in\mathcal{H}_1$ and for $\tau<0$,

$$
\begin{aligned}
\langle f|P_{\mathrm{sym}}^{0,-}(\tau)|g\rangle &= -\mathrm{i}\sum_{k=1}^N\left\langle\left(v_c^{1/2}\overline{g}\right)\phi_k\right|(\mathbb{1}_{\mathcal{H}_1}-\gamma_{0,N}^0)\mathrm{e}^{\mathrm{i}\tau(h_1-\varepsilon_k)}\left|\left(v_c^{1/2}\overline{f}\right)\phi_k\right\rangle \\
&= \langle\overline{g}|P_{\mathrm{sym}}^{0,+}(-\tau)|\overline{f}\rangle.
\end{aligned}
$$

For a bounded operator $A\in\mathcal{B}(\mathcal{H}_1)$ and for $f,g\in\mathcal{H}_1$, it holds $\langle f|Ag\rangle=\overline{\langle Ag|f\rangle}=\langle\overline{g}|\overline{A^*f}\rangle$, so that, since the functions ϕ_k are real-valued for $1\leqslant k\leqslant N$,

$$
\langle f|P_{\mathrm{sym}}^{0,-}(\tau)|g\rangle=\left\langle f\left|\overline{\left(P_{\mathrm{sym}}^{0,+}(-\tau)\right)^*\overline{g}}\right.\right\rangle. \tag{124}
$$

Since h_1 is real-valued, in the sense that $h_1 f$ is real-valued whenever f is real-valued, we easily get that

$$\forall f \in \mathcal{H}_1, \quad \overline{(\mathbb{1}_{\mathcal{H}_1} - \gamma_{0,N}^0) e^{-i\tau h_1} f} = (\mathbb{1}_{\mathcal{H}_1} - \gamma_{0,N}^0) e^{i\tau h_1} \overline{f},$$

so that,

$$\overline{\left(P_{\mathrm{sym}}^{0,+}(-\tau)\right)^* \overline{g}} = P_{\mathrm{sym}}^{0,+}(-\tau) g.$$

Together with (124), this proves $P^{0,-}(\tau) = P^{0,+}(-\tau)^*$.

6.16 Proof of Proposition 59

The expression for $\widetilde{P_{\mathrm{sym}}^0}$ in (84) comes from the expression for $\widetilde{P_{\mathrm{sym}}^0}$ in (82). Since for $k \leqslant N$, it holds $\varepsilon_k \leqslant \varepsilon_N$, we obtain

$$\forall 1 \leqslant k \leqslant N, \quad (\mathbb{1}_{\mathcal{H}_1} - \gamma_{0,N}^0)(h_1 - \varepsilon_k) \geqslant \varepsilon_{N+1} - \varepsilon_N > 0. \tag{125}$$

From (84), we deduce that $\widetilde{P_{\mathrm{sym}}^0}(i\omega)$ is a negative bounded operator for all $\omega \in \mathbb{R}_\omega$. The self-adjointness comes from Remark 57.

The bound (85) is proved similarly as in Lemma 29. Let us now prove (86). From (125), it holds that, for all $1 \leqslant k \leqslant N$,

$$0 \leqslant (\mathbb{1}_{\mathcal{H}_1} - \gamma_{0,N}^0) \frac{h_1 - \varepsilon_k}{\omega^2 + (h_1 - \varepsilon_k)^2} \leqslant \sup_{E \geqslant \varepsilon_{N+1} - \varepsilon_N} \left(\frac{E}{\omega^2 + E^2} \right) = \begin{cases} \dfrac{1}{2\omega} & \text{if } \omega \geqslant \varepsilon_{N+1} - \varepsilon_N \\[2mm] \dfrac{\varepsilon_{N+1} - \varepsilon_N}{\omega^2 + (\varepsilon_{N+1} - \varepsilon_N)^2} & \text{otherwise.} \end{cases}$$

In particular, there exists a constant $C \in \mathbb{R}^+$ such that

$$\forall 1 \leqslant k \leqslant N, \quad \forall \omega \in \mathbb{R}_\omega, \quad 0 \leqslant (\mathbb{1}_{\mathcal{H}_1} - \gamma_{0,N}^0) \frac{h_1 - \varepsilon_k}{\omega^2 + (h_1 - \varepsilon_k)^2} \leqslant \frac{C}{\sqrt{\omega^2 + 1}}.$$

Using the fact that for $1 \leqslant k \leqslant N$, ϕ_k is real-valued, with $\sum_{k=1}^N \phi_k^2 = \rho_{0,N}^0$, we obtain

$$\forall \omega \in \mathbb{R}_\omega, \quad 0 \leqslant -\widetilde{P_{\mathrm{sym}}^0}(i\omega) \leqslant \frac{2C}{\sqrt{\omega^2 + 1}} \sum_{k=1}^N v_c^{1/2} \phi_k^2 v_c^{1/2} = \frac{2C}{\sqrt{\omega^2 + 1}} v_c^{1/2} \rho_{0,N}^0 v_c^{1/2},$$

which proves (86). The fact that $v_c^{1/2} \rho_{0,N}^0 v_c^{1/2}$ is indeed a bounded self-adjoint operator on $\mathcal{H}_1$ comes from the fact that $v_c^{1/2}$ is a bounded operator from $\mathcal{C}$ to $\mathcal{H}_1$ and from $\mathcal{H}_1$ to $\mathcal{C}'$, and that the operator of multiplication by ϕ_k is a bounded operator from $\mathcal{C}'$ to $\mathcal{H}_1$ and from $\mathcal{H}_1$ to $\mathcal{C}$. Together with the fact that the function $\omega \mapsto (\omega^2 + 1)^{-1/2}$ is in $L^p(\mathbb{R}_\omega)$ for all $p > 1$, this implies that $\widetilde{P_{\mathrm{sym}}^0}(i\cdot) \in L^p(\mathbb{R}_\omega, \mathcal{S}(\mathcal{H}_1))$ for all $p > 1$. The analyticity of this map is straightforward.

6.17 Proof of Theorem 60

Let us prove the equality $2 \sum_{k=1}^N \phi_k(\mathbb{1}_{\mathcal{H}_1} - \gamma_{0,N}^0)(h_1 - \varepsilon_k)\phi_k = -\mathrm{div}\left(\rho_{0,N}^0 \nabla \cdot\right)$, as operators from $\mathcal{C}'$ to $\mathcal{C}$. We first note that, since $\phi_k \in L^4(\mathbb{R}^3)$ for $1 \leqslant k \leqslant N$, it holds $\phi_k \phi_l \in \mathcal{H}_1$ for $1 \leqslant k, l \leqslant N$. In particular,

$$\sum_{k=1}^N \phi_k \gamma_{0,N}^0 (h_1 - \varepsilon_k)\phi_k = \sum_{k=1}^N \sum_{l=1}^N |\phi_k \phi_l\rangle(\varepsilon_l - \varepsilon_k)\langle \phi_l \phi_k| = 0,$$

so that

$$2 \sum_{k=1}^N \phi_k(\mathbb{1}_{\mathcal{H}_1} - \gamma_{0,N}^0)(h_1 - \varepsilon_k)\phi_k = 2 \sum_{k=1}^N \phi_k(h_1 - \varepsilon_k)\phi_k. \tag{126}$$

Consider now $f, g \in C_c^\infty(\mathbb{R}^3, \mathbb{C})$. In view of the equality

$$(h_1 - \varepsilon_k)(\phi_k g) = \phi_k\left(-\frac{1}{2}\Delta g\right) - \nabla\phi_k \cdot \nabla g,$$

it follows that

$$2\left\langle f \left| \sum_{k=1}^N \phi_k(h_1 - \varepsilon_k)\phi_k \right| g \right\rangle_{\mathcal{H}_1} = \left\langle f \left| \sum_{k=1}^N \phi_k^2(-\Delta g) \right\rangle_{\mathcal{H}_1} - 2\left\langle f \left| \sum_{k=1}^N \phi_k \nabla\phi_k \cdot \nabla g \right\rangle_{\mathcal{H}_1}$$

$$= \langle f | \rho_{0,N}^0(-\Delta g)\rangle_{\mathcal{H}_1} - \langle f | \nabla\rho_{0,N}^0 \cdot \nabla g\rangle_{\mathcal{H}_1} = \int_{\mathbb{R}^3} \rho_{0,N}^0 \overline{\nabla f} \cdot \nabla g,$$

where we used an integration by part to obtain the last equality. Together with (126), we obtain that the operators $2\sum_{k=1}^N \phi_k(\mathbb{1}_{\mathcal{H}_1} - \gamma_{0,N}^0)(h_1 - \varepsilon_k)\phi_k$ and $-\mathrm{div}\left(\rho_{0,N}^0\nabla\cdot\right)$ are equal on the core $C_c^\infty(\mathbb{R}^3, \mathbb{C})$. The end of the proof is similar to the one of Theorem 46.

6.18 Proof of Lemma 62

It is sufficient to prove that, for any $\nu' < \varepsilon_{N+1}$, $\nu > \varepsilon_N - \nu'$, $\omega, \omega' \in \mathbb{R}_\omega$, and $f, g \in \mathcal{H}_1$, it holds

$$\mathrm{Tr}_{\mathcal{H}_1}\left(\left(v_c^{1/2}\overline{f}\right)\widetilde{G_{0,\mathrm{h}}}(\nu + \nu' + \mathrm{i}(\omega + \omega'))\left(v_c^{1/2}g\right)\widetilde{G_{0,\mathrm{p}}}(\nu' + \mathrm{i}\omega')\right)$$

$$= \mathrm{Tr}_{\mathcal{H}_1}\left(\widetilde{G_{0,\mathrm{h}}}(\nu + \nu' + \mathrm{i}(\omega + \omega'))\left(v_c^{1/2}g\right)\widetilde{G_{0,\mathrm{p}}}(\nu' + \mathrm{i}\omega')\left(v_c^{1/2}\overline{f}\right)\right)$$

We will only consider the case $\nu = 0$, $\nu' = \mu_0$, $\omega = \omega' = 0$ for simplicity, the other cases being similar. We rely on the fact that if $A, B \in \mathcal{B}(\mathcal{H}_1)$ are such that AB and BA are trace-class operators, then $\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$ [40]. In our case, we consider $f, g \in C_c^\infty \subset \mathcal{H}_1$, so that $f_1 := v_c^{1/2}f$ and $g_1 := v_c^{1/2}g$ are in $\mathcal{C}' \cap L^\infty$, and we set $A = \overline{f_1}$ and $B = \widetilde{G_{0,\mathrm{h}}}(\mu_0)g_1\widetilde{G_{0,\mathrm{p}}}(\mu_0)$. The operators A and B are bounded operators on $\mathcal{H}_1$. Moreover, from Proposition (48), we get

$$BA = \widetilde{G_{0,\mathrm{h}}}(\mu_0)g_1\widetilde{G_{0,\mathrm{p}}}(\mu_0)\overline{f_1} = \gamma_{0,N}^0\left(\frac{1}{\mu_0 - h_1}g_1\right)\left(\frac{\mathbb{1}_{\mathcal{H}_1} - \gamma_{0,N}^0}{\mu_0 - h_1}\overline{f_1}\right).$$

It holds $\gamma_{0,N}^0 \in \mathfrak{S}_1(\mathcal{H}_1)$. Also, from the definition of μ_0, it is easy to see that there exists $0 < c \leqslant C < \infty$ such that

$$c(1 - \Delta) \leqslant |\mu_0 - h_1| \leqslant C(1 - \Delta).$$

In particular, the operator $(\mu_0 - h_1)^{-1}g_1 = \left[(\mu_0 - h_1)^{-1}(1 - \Delta)\right]\left[(1 - \Delta)^{-1}g_1\right]$ is the composition of two bounded operators. Actually, the operator $(1 - \Delta)^{-1}g_1$ is in the Schatten class $\mathfrak{S}_6(\mathcal{H}_1)$, thanks to the Kato-Seiler-Simon inequality [39, 40], and it holds

$$\left\|(1-\Delta)^{-1}g_1\right\|_{\mathcal{B}(\mathcal{H}_1)} \leqslant \left\|(1-\Delta)^{-1}g_1\right\|_{\mathfrak{S}_6(\mathcal{H}_1)} \leqslant C\|g_1\|_{L^6} \leqslant C'\|g\|_{\mathcal{H}_1}, \tag{127}$$

where $C' \in \mathbb{R}^+$ is a constant independent of g. Similarly, $(\mathbb{1} - \gamma_{0,N})(\mu_0 - h_1)^{-1}\overline{f_1}$ is a bounded operator, satisfying estimates similar to (127). Altogether, we deduce that, for all $f, g \in C_c^\infty(\mathbb{R}^3)$,

$$\widetilde{G_{0,\mathrm{h}}}(\mu_0)\left(v_c^{1/2}g\right)\widetilde{G_{0,\mathrm{p}}}(\mu_0)\left(v_c^{1/2}\overline{f}\right) \in \mathfrak{S}_1(\mathcal{H}_1),$$

with

$$\left\|\widetilde{G_{0,\mathrm{h}}}(\mu_0)\left(v_c^{1/2}g\right)\widetilde{G_{0,\mathrm{p}}}(\mu_0)\left(v_c^{1/2}\overline{f}\right)\right\|_{\mathfrak{S}_1(\mathcal{H}_1)} \leqslant C\|g\|_{\mathcal{H}_1}\|f\|_{\mathcal{H}_1}, \tag{128}$$

where $C \in \mathbb{R}^+$ is a constant independent of f and g. The proof that $AB = \widetilde{G_{0,\mathrm{p}}}(\mu_0)g_1\widetilde{G_{0,\mathrm{h}}}(\mu_0)\overline{f_1}$ is trace-class is similar. As a result, we deduce that for any $f, g \in C_c^\infty$,

$$\mathrm{Tr}_{\mathcal{H}_1}\left(\left(v_c^{1/2}\overline{f}\right)\widetilde{G_{0,\mathrm{h}}}(\mu_0)\left(v_c^{1/2}g\right)\widetilde{G_{0,\mathrm{p}}}(\mu_0)\right) = \mathrm{Tr}_{\mathcal{H}_1}\left(\widetilde{G_{0,\mathrm{h}}}(\mu_0)\left(v_c^{1/2}g\right)\widetilde{G_{0,\mathrm{p}}}(\mu_0)\left(v_c^{1/2}\overline{f}\right)\right).$$

The proof for the general case $f, g \in \mathcal{H}_1$ is deduced by density from the estimate (128).

6.19 Proof of Proposition 73

Let us first prove that $\mathfrak{s}$ is a bounded linear operator. Let $\widetilde{G^{\mathrm{app}}}(\mu_0 + \mathrm{i}\cdot) \in L^2(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$. For $f, g \in \mathcal{H}_1$ and $\omega \in \mathbb{R}_\omega$,

$$\left\langle f \left| \mathfrak{s} \left[\widetilde{G^{\mathrm{app}}} \right] (\mu + \mathrm{i}\omega) \right| g \right\rangle = \langle f | K_x | g \rangle - \frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathrm{Tr}_{\mathcal{H}_1} \left(\widetilde{G^{\mathrm{app}}}(\mu_0 + \mathrm{i}(\omega + \omega')) g \widetilde{W_c^0}(\mathrm{i}\omega') \overline{f} \right) \mathrm{d}\omega'.$$

Let us first treat the exchange part K_x, and prove that it is a Hilbert-Schmidt operator. From the definition (99), K_x is an integral operator, and, from Proposition 26, its kernel satisfies

$$\int_{\mathbb{R}^3} \int_{\mathbb{R}^3} |K_x(\mathbf{r}, \mathbf{r}')|^2 \, \mathrm{d}\mathbf{r} \, \mathrm{d}\mathbf{r}' \leqslant \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\rho_{0,N}^0(\mathbf{r}) \rho_{0,N}^0(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^2} \mathrm{d}\mathbf{r} \, \mathrm{d}\mathbf{r}' < \infty,$$

where the last inequality comes from the fact that $\rho_{0,N}^0 * |\cdot|^{-2} \in L^\infty(\mathbb{R}^3)$ (since $\rho_{0,N}^0 \in L^1(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, while $|\cdot|^{-2} \in L^1(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$) and $\rho_{0,N}^0 \in L^1(\mathbb{R}^3)$. We conclude that K_x is a Hilbert-Schmidt operator, hence is bounded.

For the correlation part, we use the following lemma.

Lemma 78. *For all $f, g \in \mathcal{H}_1$ and all $\omega \in \mathbb{R}_\omega$, the operator $g \widetilde{W_c^0}(\mathrm{i}\omega) \overline{f}$ is trace-class, and*

$$\exists C \in \mathbb{R}^+, \quad \forall f, g \in \mathcal{H}_1, \quad \left\| g \widetilde{W_c^0}(\mathrm{i}\omega) \overline{f} \right\|_{\mathfrak{S}_1(\mathcal{H}_1)} \leqslant \frac{C}{(\omega^2 + 1)^{1/2}} \|f\|_{\mathcal{H}_1} \|g\|_{\mathcal{H}_1}. \tag{129}$$

Proof of Lemma 78. We first prove (129) for $f = g \in \mathcal{H}_1$. Let $\psi \in C_c^\infty(\mathbb{R}^3, \mathbb{C})$, we have

$$\left\langle \psi \left| f \widetilde{W_c^0}(\mathrm{i}\omega) \overline{f} \right| \psi \right\rangle = \left\langle \psi \left| \overline{f} v_c^{1/2} \widetilde{\chi_{\mathrm{sym}}^0}(\mathrm{i}\omega) v_c^{1/2} f \right| \psi \right\rangle,$$

and we infer from (95) that

$$\forall f \in \mathcal{H}_1, \quad \forall \omega \in \mathbb{R}_\omega, \quad \left\| f \widetilde{W_c^0}(\mathrm{i}\omega) \overline{f} \right\|_{\mathfrak{S}_1(\mathcal{H}_1)} \leqslant \frac{C}{(\omega^2 + 1)^{1/2}} \left\| f v_c \rho_{0,N}^0 v_c \overline{f} \right\|_{\mathfrak{S}_1(\mathcal{H}_1)}.$$

Since

$$\left\| f v_c \rho_{0,N}^0 v_c \overline{f} \right\|_{\mathfrak{S}_1(\mathcal{H}_1)} = \left\| \sqrt{\rho_{0,N}^0} v_c \overline{f} \right\|_{\mathfrak{S}_2(\mathcal{H}_1)}^2 = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\rho_{0,N}^0(\mathbf{r}) |f(\mathbf{r}')|^2}{|\mathbf{r} - \mathbf{r}'|^2} \, \mathrm{d}\mathbf{r} \, \mathrm{d}\mathbf{r}' \leqslant C \|f\|_{\mathcal{H}_1}^2,$$

where we used again the fact that $\rho_{0,N}^0 * |\cdot|^{-2}$ is bounded, we obtain that (129) holds true for $f = g$. For $f \neq g$, we deduce from the fact that $\widetilde{\chi_{\mathrm{sym}}^0}(\mathrm{i}\omega)$ is a bounded self-adjoint negative operator, that

$$\left\| g \widetilde{W_c^0}(\mathrm{i}\omega) \overline{f} \right\|_{\mathfrak{S}_1(\mathcal{H}_1)} = \left\| g v_c^{1/2} \widetilde{\chi_{\mathrm{sym}}^0}(\mathrm{i}\omega) v_c^{1/2} \overline{f} \right\|_{\mathfrak{S}_1(\mathcal{H}_1)} = \left\| g v_c^{1/2} \sqrt{-\widetilde{\chi_{\mathrm{sym}}^0}(\mathrm{i}\omega)} \sqrt{-\widetilde{\chi_{\mathrm{sym}}^0}(\mathrm{i}\omega)} v_c^{1/2} \overline{f} \right\|_{\mathfrak{S}_1(\mathcal{H}_1)}$$

$$\leqslant \left\| g v_c^{1/2} \sqrt{-\widetilde{\chi_{\mathrm{sym}}^0}(\mathrm{i}\omega)} \right\|_{\mathfrak{S}_2(\mathcal{H}_1)} \left\| \sqrt{-\widetilde{\chi_{\mathrm{sym}}^0}(\mathrm{i}\omega)} v_c^{1/2} \overline{f} \right\|_{\mathfrak{S}_2(\mathcal{H}_1)}$$

$$\leqslant \left\| g v_c^{1/2} \widetilde{\chi_{\mathrm{sym}}^0}(\mathrm{i}\omega) v_c^{1/2} \overline{g} \right\|_{\mathfrak{S}_1(\mathcal{H}_1)}^{1/2} \left\| f v_c^{1/2} \widetilde{\chi_{\mathrm{sym}}^0}(\mathrm{i}\omega) v_c^{1/2} \overline{f} \right\|_{\mathfrak{S}_1(\mathcal{H}_1)}^{1/2}$$

$$\leqslant \frac{C}{(\omega^2 + 1)^{1/2}} \|f\|_{\mathcal{H}_1} \|g\|_{\mathcal{H}_1}.$$

$\square$

We now proceed to the proof of Proposition 73. From Lemma 78, we get, for $f, g \in \mathcal{H}_1$,

$$\left| \left\langle f \left| \mathfrak{s}_c \left[\widetilde{G^{\mathrm{app}}} \right] (\mu + \mathrm{i}\omega) \right| g \right\rangle \right| = \frac{1}{2\pi} \left| \int_{-\infty}^{+\infty} \mathrm{Tr}_{\mathcal{H}_1} \left(\widetilde{G^{\mathrm{app}}}(\mu_0 + \mathrm{i}(\omega + \omega')) g \widetilde{W^0}(\mathrm{i}\omega') \overline{f} \right) \mathrm{d}\omega' \right|$$

$$\leqslant \frac{1}{2\pi} \int_{-\infty}^{+\infty} \left\| \widetilde{G^{\mathrm{app}}}(\mu_0 + \mathrm{i}(\omega + \omega')) \right\|_{\mathcal{B}(\mathcal{H}_1)} \left\| g \widetilde{W^0}(\mathrm{i}\omega') \overline{f} \right\|_{\mathfrak{S}_1(\mathcal{H}_1)} \mathrm{d}\omega'$$

$$\leqslant \int_{-\infty}^{+\infty} \left\| \widetilde{G^{\mathrm{app}}}(\mu_0 + \mathrm{i}(\omega + \omega')) \right\|_{\mathcal{B}(\mathcal{H}_1)} \frac{C}{(\omega'^2 + 1)^{1/2}} \|f\|_{\mathcal{H}_1} \|g\|_{\mathcal{H}_1} \mathrm{d}\omega'$$

$$\leqslant C' \left\| \widetilde{G^{\mathrm{app}}}(\mu_0 + \mathrm{i}\cdot) \right\|_{L^2(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))} \|f\|_{\mathcal{H}_1} \|g\|_{\mathcal{H}_1},$$

where we used Cauchy-Schwarz inequality for the last inequality and the fact that $\omega \mapsto (\omega^2 + 1)^{-1/2} \in L^2(\mathbb{R}_\omega)$. Here, C' does not depend on $\omega \in \mathbb{R}_\omega$ nor on $f, g \in \mathcal{H}_1$. Altogether, we deduce that $\mathfrak{s}$ is a bounded linear operator from $L^2(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$ to $L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$.

We now prove the claimed properties of $\mathfrak{g}_\lambda$. Consider $M > 0$. By definition of μ_0, the real number $d := \max(\varepsilon_{N+1} - \mu_0, \mu_0 - \varepsilon_N)$ is positive, and $|\mu_0 - h_1| \geqslant d$. Let us choose $0 < \lambda_M < d/M$. For $0 \leqslant \lambda \leqslant \lambda_M$ and $\widetilde{\Sigma^{\mathrm{app}}}(\mu_0 + \mathrm{i}\cdot) \in L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$ such that $\left\| \widetilde{\Sigma^{\mathrm{app}}}(\mu_0 + \mathrm{i}\cdot) \right\|_{L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))} \leqslant M$, it holds

$$\forall \omega \in \mathbb{R}_\omega, \quad \mu_0 + \mathrm{i}\omega - h_1 - \lambda \widetilde{\Sigma^{\mathrm{app}}}(\mu_0 + \mathrm{i}\omega) = [\mu_0 + \mathrm{i}\omega - h_1] \left(1 - \lambda [\mu_0 + \mathrm{i}\omega - h_1]^{-1} \widetilde{\Sigma^{\mathrm{app}}}(\mu_0 + \mathrm{i}\omega) \right).$$

Since

$$\left\| \lambda [\mu_0 + \mathrm{i}\omega - h_1]^{-1} \widetilde{\Sigma^{\mathrm{app}}}(\mu_0 + \mathrm{i}\omega) \right\|_{\mathcal{B}(\mathcal{H}_1)} \leqslant \frac{\lambda}{d} \left\| \widetilde{\Sigma^{\mathrm{app}}}(\mu_0 + \mathrm{i}\omega) \right\|_{\mathcal{B}(\mathcal{H}_1)} \leqslant \frac{\lambda}{d} M \leqslant \frac{\lambda_M}{d} M < 1,$$

the operator $1 - \lambda [\mu_0 + \mathrm{i}\omega - h_1]^{-1} \widetilde{\Sigma^{\mathrm{app}}}(\mu_0 + \mathrm{i}\omega)$ is invertible, with

$$\left\| \left(1 - \lambda [\mu_0 + \mathrm{i}\omega - h_1]^{-1} \widetilde{\Sigma^{\mathrm{app}}}(\mu_0 + \mathrm{i}\omega) \right)^{-1} \right\|_{\mathcal{B}(\mathcal{H}_1)} \leqslant \frac{d}{d - \lambda_M M}.$$

Since $\mu_0 + \mathrm{i}\omega - h_1$ is an invertible operator with $\left\| (\mu_0 + \mathrm{i}\omega - h_1)^{-1} \right\|_{\mathcal{B}(\mathcal{H}_1)} \leqslant (\omega^2 + d^2)^{1/2}$, we obtain that $\mu_0 + \mathrm{i}\omega - h_1 - \lambda \widetilde{\Sigma^{\mathrm{app}}}(\mu_0 + \mathrm{i}\omega)$ is invertible, with

$$\left\| \left[\mu_0 + \mathrm{i}\omega - h_1 - \lambda \widetilde{\Sigma^{\mathrm{app}}}(\mu_0 + \mathrm{i}\omega) \right]^{-1} \right\|_{\mathcal{B}(\mathcal{H}_1)} \leqslant \frac{d}{d - \lambda_M M} \left\| (\mu_0 + \mathrm{i}\omega - h_1)^{-1} \right\|_{\mathcal{B}(\mathcal{H}_1)} \leqslant \frac{K_M}{(\omega^2 + 1)^{1/2}}.$$

We deduce from this inequality that

$$\left\| \mathfrak{g}_\lambda \left(\widetilde{\Sigma^{\mathrm{app}}} \right) (\mu_0 + \mathrm{i}\cdot) \right\|_{L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))} + \left\| \mathfrak{g}_\lambda \left(\widetilde{\Sigma^{\mathrm{app}}} \right) (\mu_0 + \mathrm{i}\cdot) \right\|_{L^2(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))} \leqslant C_M,$$

where the constant $C_M \in \mathbb{R}^+$ does not depend on $\lambda \in [0, \lambda_M]$. This gives the claimed result. Finally, (102) is a direct consequence of the resolvent formula.

6.20 Proof of Theorem 74

Let us denote for simplicity

$$\|\mathfrak{s}\| = \|\mathfrak{s}\|_{\mathcal{B}(L^2(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1)), L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1)))},$$

and fix $M > \|\mathfrak{s}\| \left\| \widetilde{G^0}(\mu + \mathrm{i}\cdot) \right\|_{L^2(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))}$. Let λ_M and C_M be chosen as in Proposition 73 for this choice of $M > 0$, and introduce

$$r = \frac{M}{\|s\|} - \left\| \widetilde{G^0}(\mu + \mathrm{i}\cdot) \right\|_{L^2(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))} > 0.$$

For this choice of r, it holds that, for any $\widetilde{G^{\mathrm{app}}} \in \mathfrak{B}\left(\widetilde{G_0}, r\right)$,

$$\left\|\mathfrak{s}\left[\widetilde{G^{\mathrm{app}}}\right](\mu_0 + \mathrm{i}\cdot)\right\|_{L^\infty(\mathbb{R}_\omega, \mathfrak{B}(\mathcal{H}_1))} \leqslant M.$$

Therefore, from Proposition 73, $\mathfrak{g}_\lambda \circ \mathfrak{s}\left[\widetilde{G^{\mathrm{app}}}\right]$ is well-defined for all $\lambda \in [0, \lambda_M]$.

Let us prove that there exists $\lambda_* > 0$ sufficiently small such that for any $0 \leqslant \lambda \leqslant \lambda_*$, $\mathfrak{g}_\lambda \circ \mathfrak{s}$ maps $\mathfrak{B}\left(\widetilde{G^0}, r\right)$ into itself. For $\widetilde{G^{\mathrm{app}}} \in \mathfrak{B}\left(\widetilde{G_0}, r\right)$, it holds

$$\left\|\left(\mathfrak{g}_\lambda \circ \mathfrak{s}\left[\widetilde{G^{\mathrm{app}}}\right] - \widetilde{G_0}\right)(\mu_0 + \mathrm{i}\cdot)\right\|_{L^2(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))}$$

$$\leqslant \left\|\left(\mathfrak{g}_\lambda \circ \mathfrak{s}\left[\widetilde{G^{\mathrm{app}}}\right] - \mathfrak{g}_\lambda \circ \mathfrak{s}\left[\widetilde{G_0}\right]\right)(\mu_0 + \mathrm{i}\cdot)\right\|_{L^2(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))} \tag{130}$$

$$+ \left\|\left(\mathfrak{g}_\lambda \circ \mathfrak{s}\left[\widetilde{G_0}\right] - \widetilde{G^0}\right)(\mu_0 + \mathrm{i}\cdot)\right\|_{L^2(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))}. \tag{131}$$

To control the first term (130), we use the following result.

Lemma 79. *The map $\mathfrak{g}_\lambda \circ \mathfrak{s}$ is $(\lambda C_M^2 \|\mathfrak{s}\|)$-Lipschitz on $\mathfrak{B}\left(\widetilde{G_0}, r\right)$.*

Proof of Lemma 79. Let $\widetilde{G_1^{\mathrm{app}}}, \widetilde{G_2^{\mathrm{app}}} \in \mathfrak{B}\left(\widetilde{G_0}, r\right)$. From (102), we obtain

$$\mathfrak{g}_\lambda \circ \mathfrak{s}\left[\widetilde{G_1^{\mathrm{app}}}\right] - \mathfrak{g}_\lambda \circ \mathfrak{s}\left[\widetilde{G_2^{\mathrm{app}}}\right] = \lambda\left(\mathfrak{g}_\lambda \circ \mathfrak{s}\left[\widetilde{G_1^{\mathrm{app}}}\right]\right)\left(\mathfrak{s}\left[\widetilde{G_2^{\mathrm{app}}}\right] - \mathfrak{s}\left[\widetilde{G_1^{\mathrm{app}}}\right]\right)\left(\mathfrak{g}_\lambda \circ \mathfrak{s}\left[\widetilde{G_2^{\mathrm{app}}}\right]\right). \tag{132}$$

From Proposition 73,

$$\left\|\mathfrak{g}_\lambda \circ \mathfrak{s}\left[\widetilde{G_j^{\mathrm{app}}}\right](\mu_0 + \mathrm{i}\cdot)\right\|_{L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))} \leqslant C_M \quad \text{for} \quad 1 \leqslant j \leqslant 2.$$

Moreover,

$$\left\|\left(\mathfrak{s}\left[\widetilde{G_2^{\mathrm{app}}}\right] - \mathfrak{s}\left[\widetilde{G_1^{\mathrm{app}}}\right]\right)(\mu_0 + \mathrm{i}\cdot)\right\|_{L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1)} \leqslant \|\mathfrak{s}\|\left\|\left(\widetilde{G_2^{\mathrm{app}}} - \widetilde{G_1^{\mathrm{app}}}\right)(\mu_0 + \mathrm{i}\cdot)\right\|_{L^2(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))}.$$

Plugging these estimates into (132), we obtain

$$\left\|\left(\mathfrak{g}_\lambda \circ \mathfrak{s}\left[\widetilde{G_1^{\mathrm{app}}}\right] - \mathfrak{g}_\lambda \circ \mathfrak{s}\left[\widetilde{G_2^{\mathrm{app}}}\right]\right)(\mu_0 + \mathrm{i}\cdot)\right\|_{L^2(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))}$$

$$\leqslant \lambda C_M^2 \|\mathfrak{s}\|\left\|\left(\widetilde{G_2^{\mathrm{app}}} - \widetilde{G_1^{\mathrm{app}}}\right)(\mu_0 + \mathrm{i}\cdot)\right\|_{L^2(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))},$$

which proves that $\mathfrak{g}_\lambda \circ \mathfrak{s}$ is $(\lambda C_M^2 \|\mathfrak{s}\|)$-Lipschitz on $\mathfrak{B}\left(\widetilde{G_0}, r\right)$. $\qquad\square$

Let us now control (131). By noting that $\mathfrak{g}_{\lambda=0} \circ \mathfrak{s}\left[\widetilde{G_0}\right] = \widetilde{G_0}$, we get from the resolvent formula that

$$\mathfrak{g}_\lambda \circ \mathfrak{s}\left[\widetilde{G_0}\right] - \widetilde{G_0} = (\mathfrak{g}_\lambda - \mathfrak{g}_0) \circ \mathfrak{s}\left(\widetilde{G_0}\right) = \lambda\left(\mathfrak{g}_\lambda \circ \mathfrak{s}\left[\widetilde{G_0}\right]\right)\left(\mathfrak{s}\left[\widetilde{G_0}\right]\right)\widetilde{G_0}.$$

Using estimates similar to the ones used in the proof of Lemma 79, we deduce that

$$\left\|\left(\mathfrak{g}_\lambda \circ \mathfrak{s}\left[\widetilde{G_0}\right] - \widetilde{G_0}\right)(\mu_0 + \mathrm{i}\cdot)\right\|_{L^2(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))} \leqslant \lambda C_M^2 \left\|\mathfrak{s}\left[\widetilde{G_0}\right](\mu_0 + \mathrm{i}\cdot)\right\|_{L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))}. \tag{133}$$

From Lemma 79 and (133), we arrive at the conclusion that for all $0 \leqslant \lambda \leqslant \lambda_*$, where

$$\lambda_* = \frac{1}{C_M^2\left(\|\mathfrak{s}\| r + \left\|\mathfrak{s}\left[\widetilde{G_0}\right](\mu_0 + \mathrm{i}\cdot)\right\|_{L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))}\right)},$$

it holds $\mathfrak{g}_\lambda \circ \mathfrak{s} \left(\mathfrak{B} \left(\widetilde{G_0}, r \right) \right) \subset \mathfrak{B} \left(\widetilde{G_0}, r \right)$.

Finally, without loss of generality, we can assume that $\lambda_* C_M^2 \|\mathfrak{s}\| < 1$, so that, from Lemma 79, we get that for all $0 \leqslant \lambda \leqslant \lambda_*$, the map $\mathfrak{g}_\lambda \circ \mathfrak{s}$ is a contraction. The end of the proof follows from Picard's fixed point theorem.

Acknowledgements

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